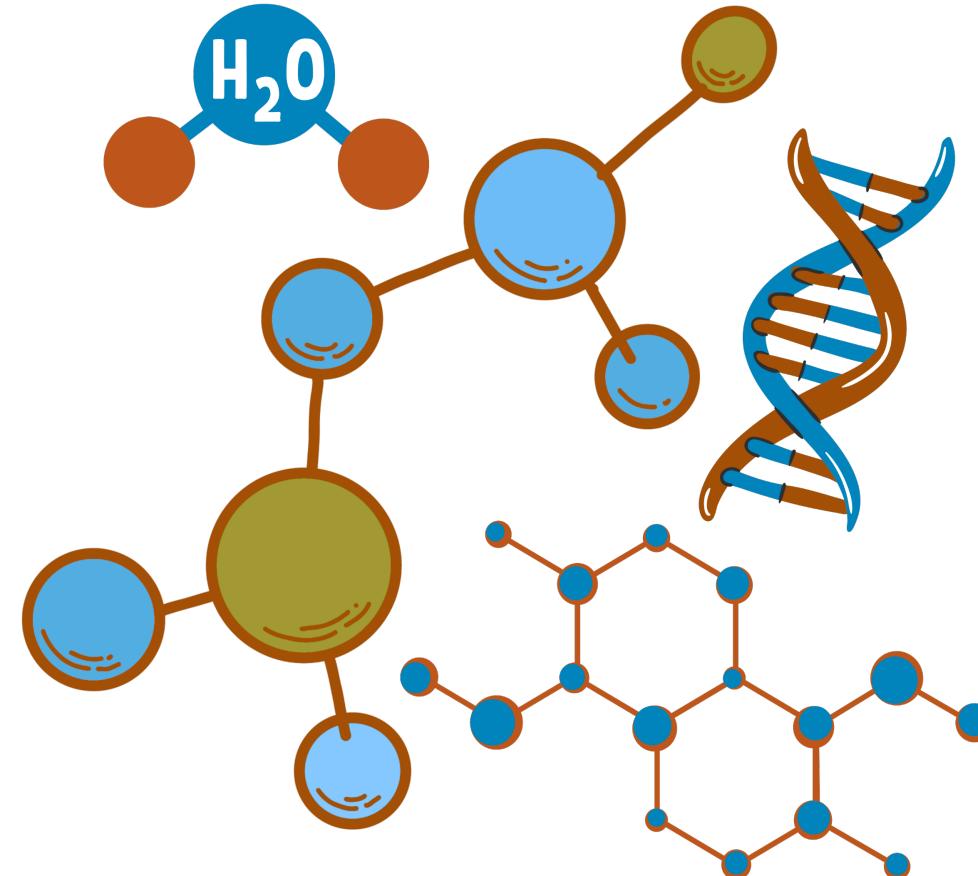


Chapter 1: Introduction to Organic Chemistry



1. Origins and Scope of Organic Chemistry

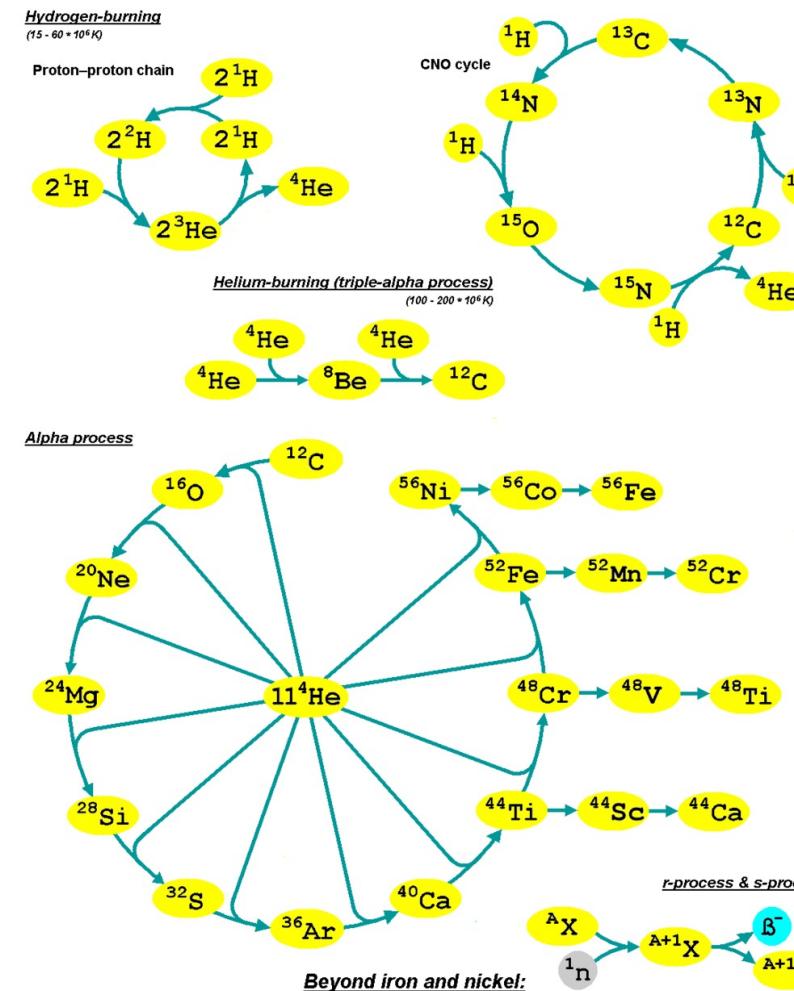
1.1 Life and the Chemistry of Carbon Compounds.

■ Why Carbon?

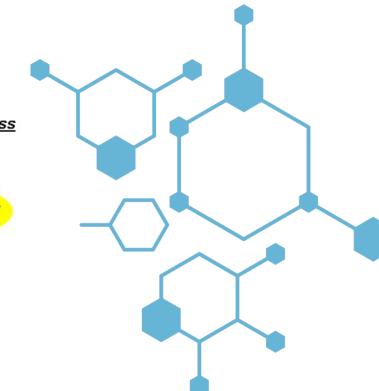
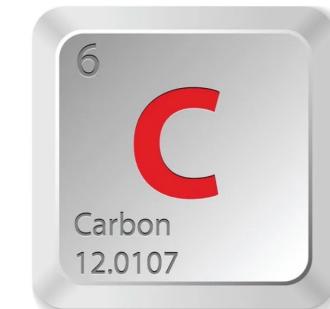
- Basis of organic chemistry (carbon compounds).
- Carbon forms strong and diverse bonds:
 - With itself → form long chains and rings.
 - With H, N, O, S → form wide variety of compounds.
 - Central to life's molecular structure compared with silicon-based life molecules (weaker bonds).

■ Origin of Carbon

- Light elements (H, He) formed in the Big Bang.
- Heavier elements (like carbon) formed in stars through nuclear fusion and released during supernova explosions.



Ref:
Narlikar (1995), From Black Clouds to Black Holes
Pappas, S. (2022). Carbon facts. Live Science.



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.
- Believed synthesis required a mysterious “vital force.”
- Inorganic compounds = substances from nonliving sources.

2- Wöhler's Discovery (1828)

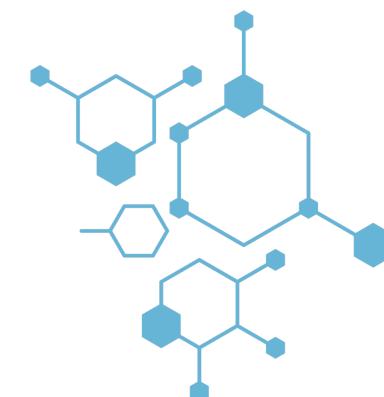
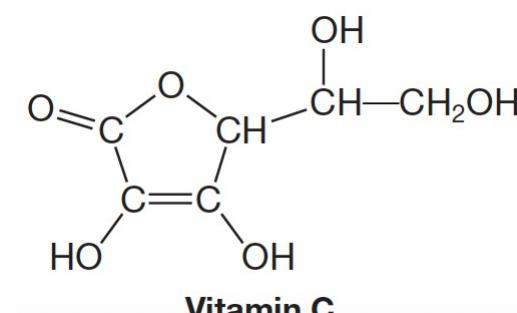
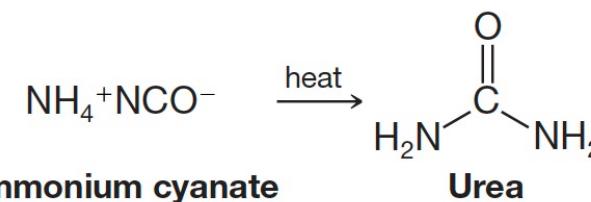
- Friedrich Wöhler synthesized urea (organic, from urine) from ammonium cyanate (inorganic).
- Proved that organic compounds can be synthesized from inorganic precursors.
- Marked the beginning of organic chemistry as a true scientific discipline.

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.



Chapter 1: Introduction to Organic Chemistry

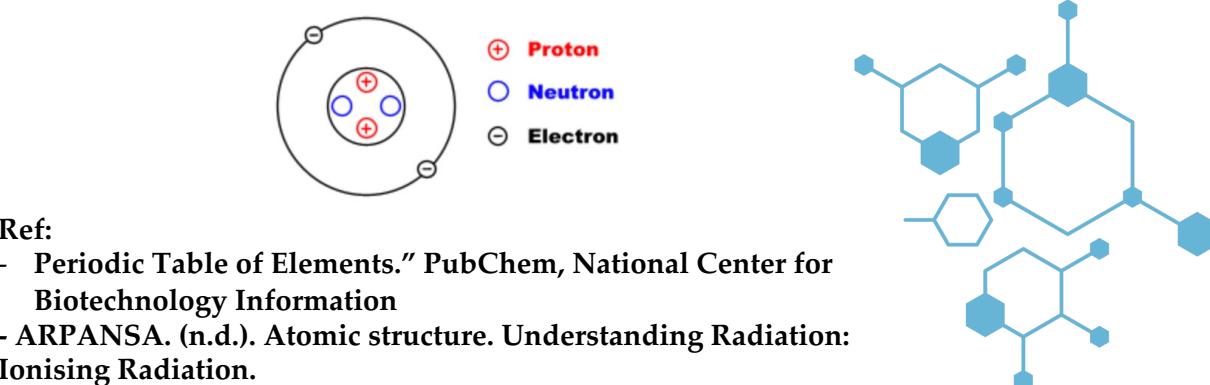
2. Atomic structure, Electron Configuration, and Molecular Orbitals

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.

The image shows the periodic table of elements, highlighting the first 18 groups. The table includes element symbols, atomic numbers, and atomic masses. A legend at the top right explains the symbols: 1 IA (H), 2 IIA (He), 6 IVA (C), 13 IIIA (Al), 14 IVA (Si), 15 VA (P), 16 VIA (S), 17 VIIA (Cl), and 18 VIIIA (Ar). The table is color-coded by group: 1 IA (pink), 2 IIA (light blue), 13 IIIA (light blue), 14 IVA (light blue), 15 VA (light blue), 16 VIA (light blue), 17 VIIA (light blue), and 18 VIIIA (light blue). The remaining groups (3-12, 19-36, 37-54, 55-86, 87-118) are in their standard grey/black colors.

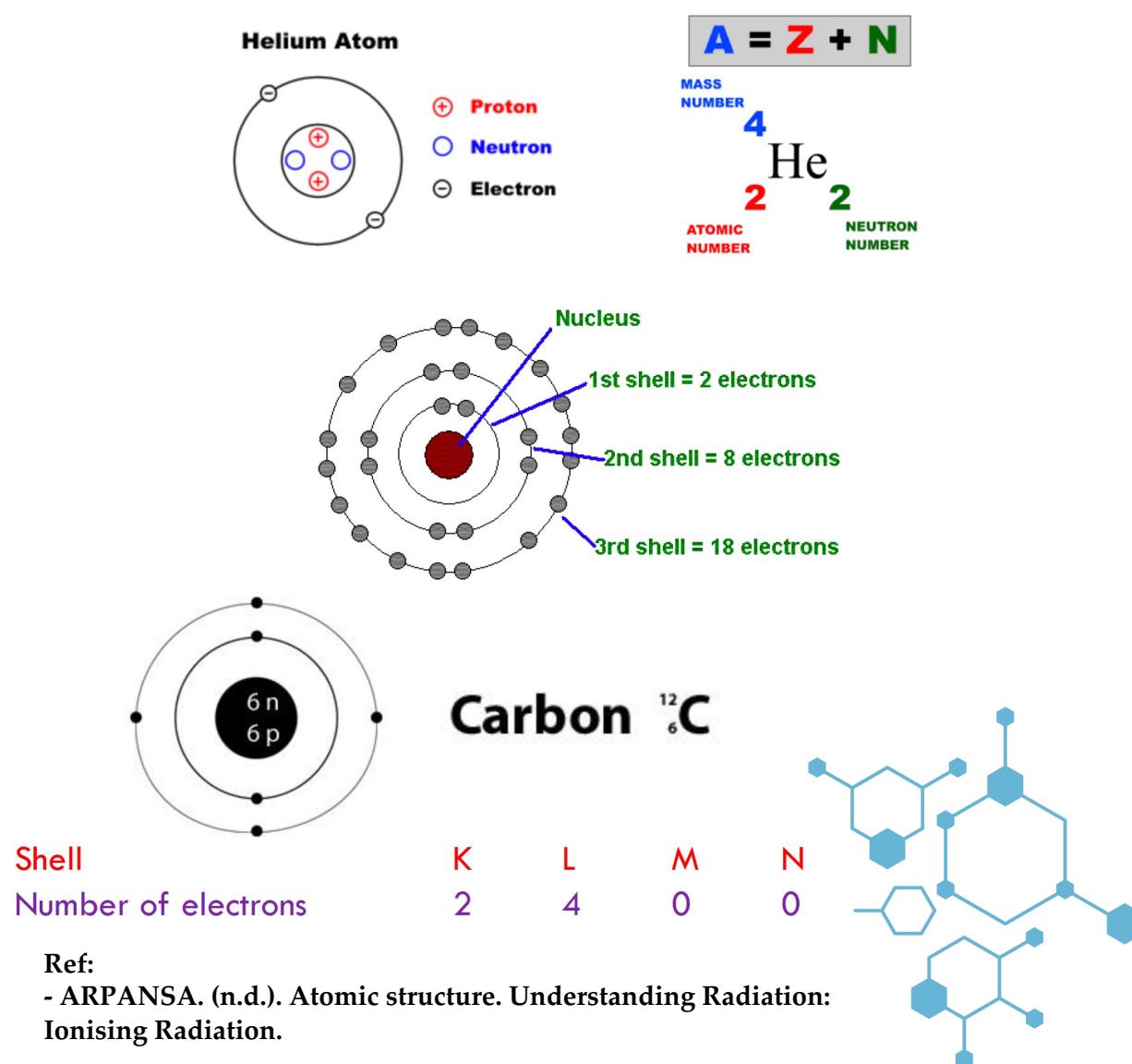
1 IA	2 IIA	6 IVA	13 IIIA	14 IVA	15 VA	16 VIA	17 VIIA	18 VIIIA
1 H Hydrogen 1.0079	2 Be Beryllium 9.0122	6 C Carbon 12.011	13 Al Aluminum 26.982	14 Si Silicon 28.086	15 P Phosphorus 30.974	16 S Sulfur 32.065	17 Cl Chlorine 35.453	18 He Helium 4.0026
3 Li Lithium 6.941	4 Be Beryllium 9.0122	11 Na Sodium 22.990	12 Mg Magnesium 24.305	3 IIIB Sc Scandium 44.956	4 IVB Ti Titanium 47.867	5 VB V Vanadium 50.942	6 VIB Cr Chromium 51.996	7 VIIB Mn Manganese 54.938
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
37 Rb Rubidium 85.468	38 Sr Strontium 87.62	39 Y Yttrium 88.906	40 Zr Zirconium 91.224	41 Nb Niobium 92.905	42 Mo Molybdenum 95.94	43 Tc Technetium (98)	44 Ru Ruthenium 101.07	45 Rh Rhodium 102.91
55 Cs Cesium 132.91	56 Ba Barium 137.33	57 *La Lanthanum 138.91	58 Hf Hafnium 178.49	59 Ta Tantalum 180.95	60 W Tungsten 183.84	61 Re Rhenium 186.21	62 Os Osmium 190.23	63 Ir Iridium 192.22
87 Fr Francium (223)	88 Ra Radium (226)	89 #Ac Actinium (227)	104 Rf Rutherfordium (261)	105 Db Dubnium (262)	106 Sg Seaborgium (266)	107 Bh Bohrium (264)	108 Hs Hassium (277)	109 Mt Meitnerium (268)
*Lanthanide Series			58 Ce Cerium 140.12	59 Pr Praseodymium 140.91	60 Nd Neodymium 144.24	61 Pm Promethium (145)	62 Sm Samarium 150.36	63 Eu Europium 151.96
# Actinide Series			90 Th Thorium 232.04	91 Pa Protactinium 231.04	92 U Uranium 238.03	93 Np Neptunium (237)	94 Pu Plutonium (244)	95 Am Americium (243)
# Actinide Series			96 Cm Curium (247)	97 Bk Berkelium (247)	98 Cf Californium (251)	99 Es Einsteinium (252)	100 Fm Fermium (257)	101 Md Mendelevium (258)
# Actinide Series			102 No Nobelium (259)	103 Lr Lawrencium (262)	104 Hf Hafnium (264)	105 Ta Tantalum (268)	106 W Tungsten (277)	107 Re Rhenium (281)



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 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.



Chapter 1: Introduction to Organic Chemistry

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 ($_6\text{C}$) – group #4 = 4 valence electrons
 - Oxygen ($_8\text{O}$) – group #6 = 6 valence electrons
 - Halogens (X) – group #7 = 7 valence electrons

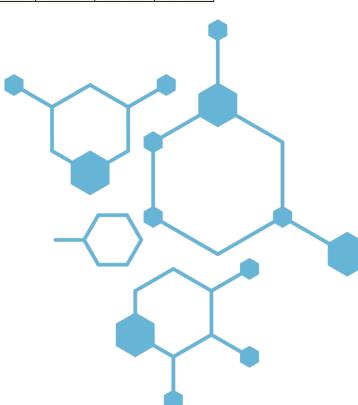
Atomic number → Symbol → Name (IUPAC) → Atomic mass →

IUPAC recommendations: → Chemical Abstracts Service group notation: →

1	IA	1	IIA	6	IIIA	13	IVA	14	VIA	15	VA	16	VIA	17	VIIA	18	VIIIA		
	H Hydrogen 1.0079		Be Beryllium 9.0122		C Carbon 12.011										He Helium 4.0026				
3	Li Lithium 6.941	11	Mg Magnesium 24.305	19	K Potassium 39.098	37	Rb Rubidium 85.468	55	Cs Cesium 132.91	87	Fr Francium (223)	58	Ce Cerium 140.12	90	Th Thorium 232.04	59	Pr Praseodymium 140.91	91	Pa Protactinium 231.04
4	Be Beryllium 9.0122	12	Mg Magnesium 24.305	20	Ca Calcium 40.078	38	Sr Strontium 87.62	56	Ba Barium 137.33	88	Ra Radium (226)	104	#Ac Actinium (227)	105	Rf Rutherfordium (261)	106	Db Dubnium (262)	107	Sg Seaborgium (266)
5		13	Sc Scandium 44.956	21	Ti Titanium 47.867	39	Y Yttrium 88.906	57	*La Lanthanum 138.91	89	Ra Radium (226)	104	Rf Rutherfordium (261)	105	Db Dubnium (262)	106	Sg Seaborgium (266)	107	Bh Bohrium (264)
6		14	V Vanadium 50.942	22	Cr Chromium 51.996	40	Zr Zirconium 91.224	72	Hf Hafnium 178.49	73	Ta Tantalum 180.95	74	W Tungsten 183.84	75	Re Rhenium 195.94	76	Os Osmium 186.21	77	Ir Iridium 190.23
7		15	Mn Manganese 54.938	23	Cr Chromium 51.996	41	Nb Niobium 92.905	43	Tc Technetium (98)	42	Mo Molybdenum 95.94	44	Ru Ruthenium 101.07	45	Fe Iron 55.845	46	Co Cobalt 58.933	47	Rh Rhodium 102.91
8		16	Fe Iron 55.845	24	Mn Manganese 54.938	48	Tc Technetium (98)	78	Ni Nickel 58.693	29	Co Cobalt 63.546	30	Cu Copper 65.409	31	Zn Zinc 65.409	32	Ge Germanium 69.723	33	As Arsenic 74.922
9		17	Co Cobalt 58.693	25	Mn Manganese 54.938	49	Rh Rhodium 102.91	79	Pt Platinum 195.08	27	Co Cobalt 58.693	80	Hg Mercury 200.59	81	Tl Thallium 195.08	82	Pb Lead 207.2	83	Bi Bismuth 208.98
10		18	Ni Nickel 63.546	26	Cr Chromium 51.996	50	Pd Palladium 106.42	80	Au Gold 196.97	28	Co Cobalt 63.546	81	Hg Mercury 200.59	84	Po Polonium (209)	85	At Astatine (210)	86	Rn Radon (222)
11		19	Cr Chromium 51.996	27	Mn Manganese 54.938	51	Fe Iron 55.845	82	Pt Platinum 195.08	29	Co Cobalt 63.546	83	Tl Thallium 204.38	84	Bi Bismuth (209)	85	At Astatine (210)	86	Rn Radon (222)
12		20	Mn Manganese 54.938	28	Fe Iron 55.845	52	Rh Rhodium 102.91	83	Au Gold 196.97	30	Zn Zinc 65.409	84	Tl Thallium 204.38	85	Po Polonium (209)	86	Rn Radon (222)	87	Kr Krypton 83.798
13		21	Cr Chromium 51.996	29	Mn Manganese 54.938	53	Rh Rhodium 102.91	85	Hg Mercury 200.59	31	Zn Zinc 65.409	86	Bi Bismuth 208.98	87	Po Polonium (209)	88	At Astatine (210)	89	Rn Radon (222)
14		22	Cr Chromium 51.996	30	Fe Iron 55.845	54	Pd Palladium 106.42	87	Au Gold 196.97	32	Ge Germanium 72.64	88	Bi Bismuth 208.98	89	Po Polonium (209)	90	At Astatine (210)	91	Rn Radon (222)
15		23	Cr Chromium 51.996	33	Co Cobalt 63.546	55	Pd Palladium 106.42	88	Hg Mercury 200.59	33	As Arsenic 78.96	89	Bi Bismuth 208.98	90	Po Polonium (209)	91	At Astatine (210)	92	Rn Radon (222)
16		24	Cr Chromium 51.996	34	Co Cobalt 63.546	56	Pd Palladium 106.42	89	Au Gold 196.97	34	Se Selenium 78.96	90	Bi Bismuth 208.98	91	Po Polonium (209)	92	At Astatine (210)	93	Rn Radon (222)
17		25	Cr Chromium 51.996	35	Co Cobalt 63.546	57	Pd Palladium 106.42	90	Hg Mercury 200.59	35	Cl Chlorine 35.453	91	Bi Bismuth 208.98	92	Po Polonium (209)	93	At Astatine (210)	94	Rn Radon (222)
18		26	Cr Chromium 51.996	36	Co Cobalt 63.546	58	Pd Palladium 106.42	91	Hg Mercury 200.59	36	Ar Argon 39.948	92	Bi Bismuth 208.98	93	Po Polonium (209)	94	At Astatine (210)	95	Rn Radon (222)

Ref:

- Periodic Table of Elements." PubChem, National Center for Biotechnology Information
- ARPANSA. (n.d.). Atomic structure. Understanding Radiation: Ionising Radiation.

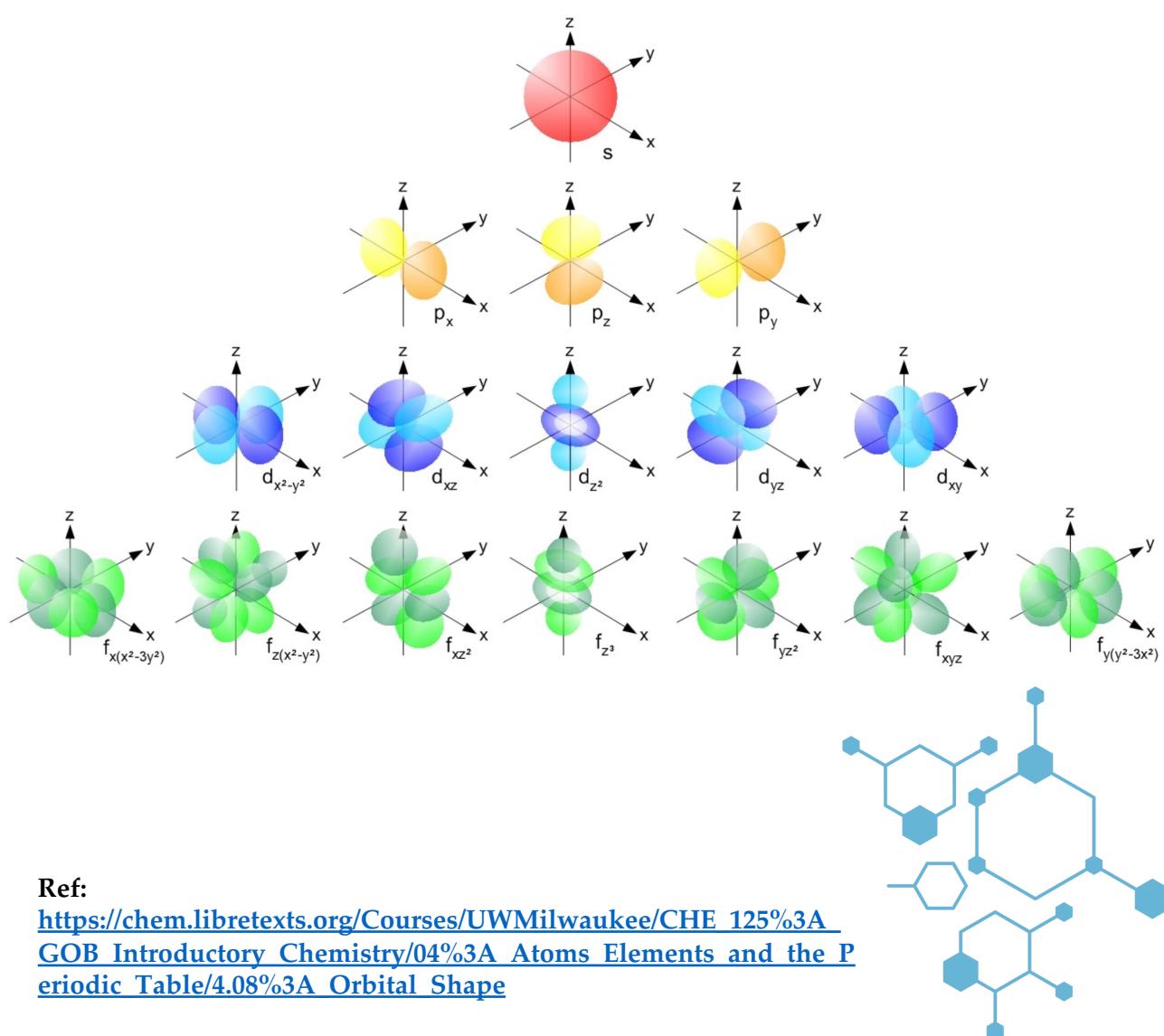


2. Atomic structure, Electron Configuration, and Molecular Orbitals

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.

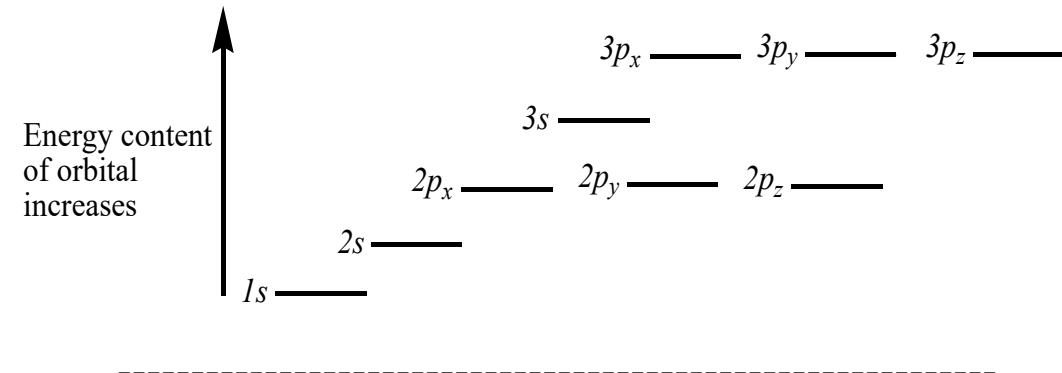


2. Atomic structure, Electron Configuration, and Molecular Orbitals

2.2 Atomic orbitals and electron configuration

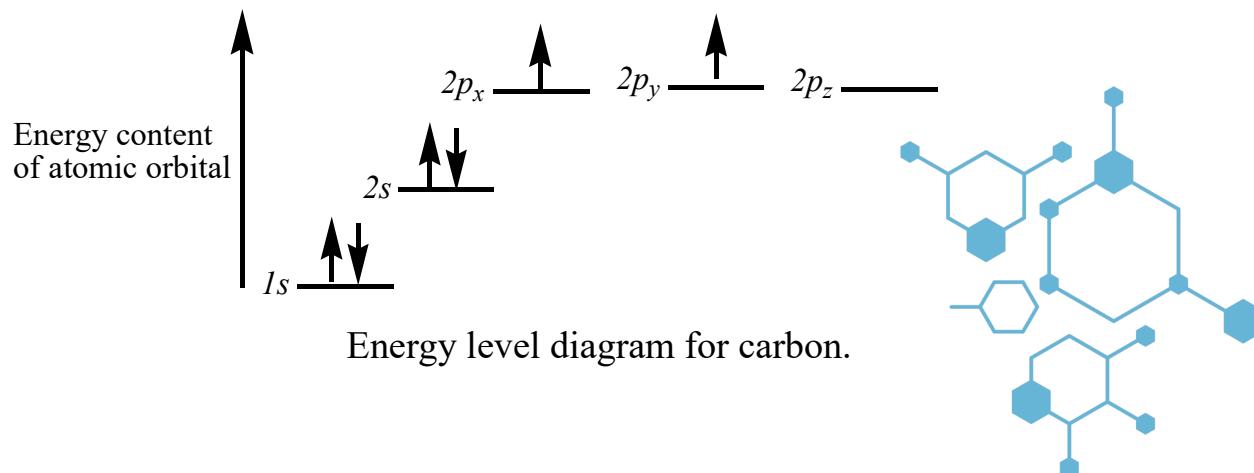
▪ Atomic Orbitals

- Each energy shell has specific numbers and types of the atomic orbitals. For example:
 - K shell has only one (1s) orbital.
 - L shell has one (2s) and three (2p) 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 least one electron (*Hund's Rule*).



➤ Filling atomic orbitals of carbon atom (₆C):

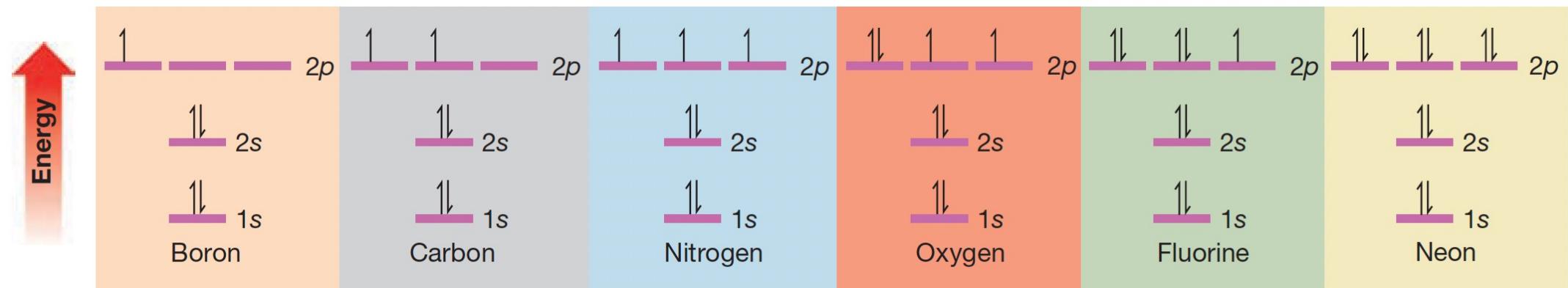
$1s^2 2s^2 2p1x2p1y$ or $1s^2 2s^2 2p^2$



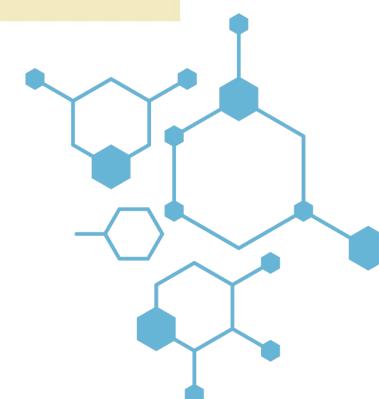
2. Atomic structure, Electron Configuration, and Molecular Orbitals

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.



Ref:
The textbook

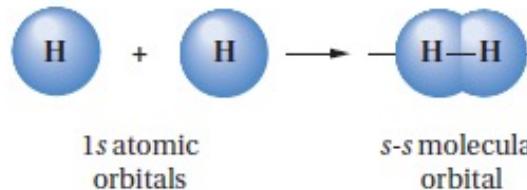


2. Atomic structure, Electron Configuration, and Molecular Orbitals

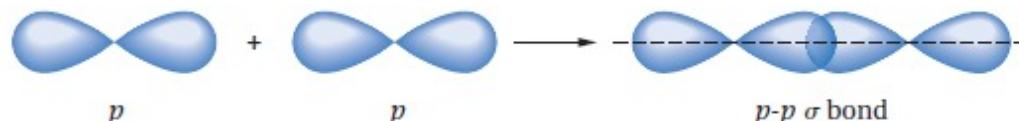
2.3 Molecular Orbitals (MOs)

- Molecular orbitals are formed as a result of overlapping two molecular 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.

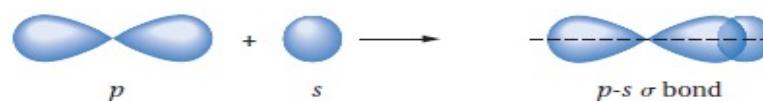
- Two (**s**) atomic orbitals overlap:



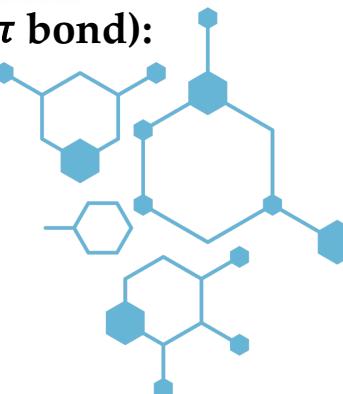
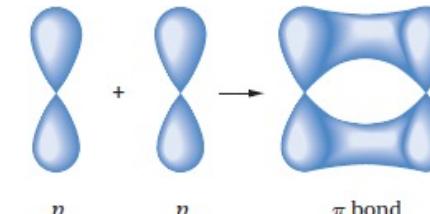
- Two (*p*) atomic orbitals overlap to form (σ bond):



- (s) and (p) atomic orbitals overlap:



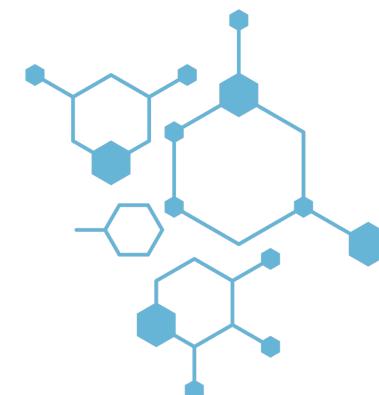
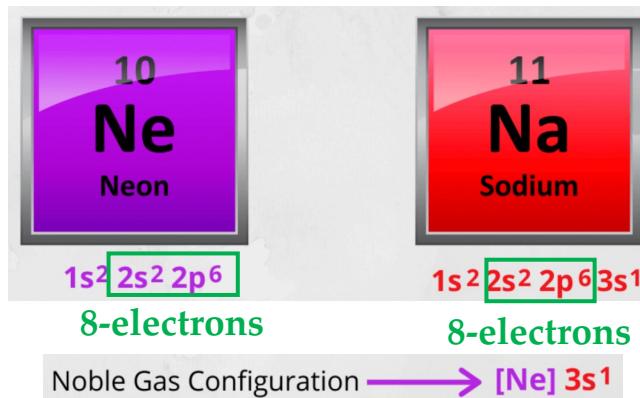
- Two (p) atomic orbitals overlap to form (π bond):



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 trend 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.



Ref: <https://sciencenotes.org>

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*).

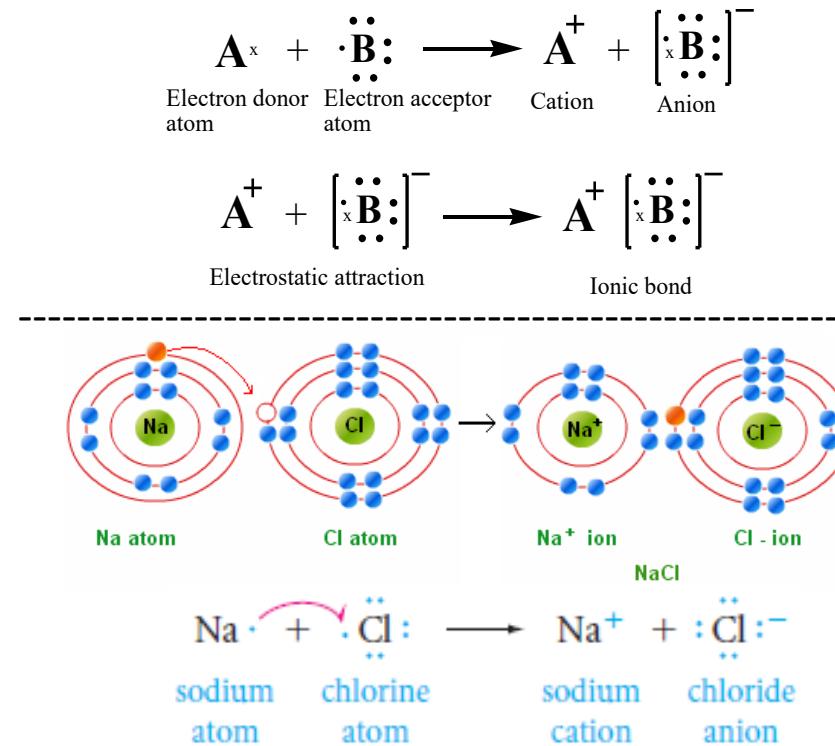
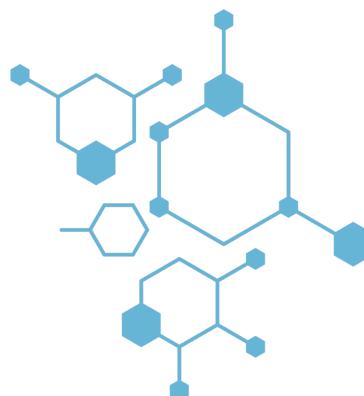


TABLE 1.1 ELECTRONEGATIVITIES OF SOME OF THE ELEMENTS

Increasing electronegativity \rightarrow

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

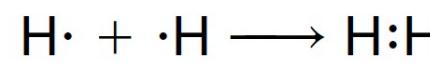
Increasing electronegativity



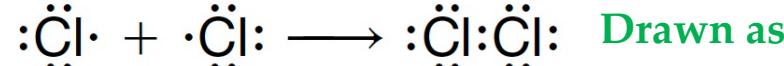
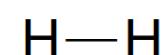
3. Chemical Bonding

3.3 Covalent Bonds

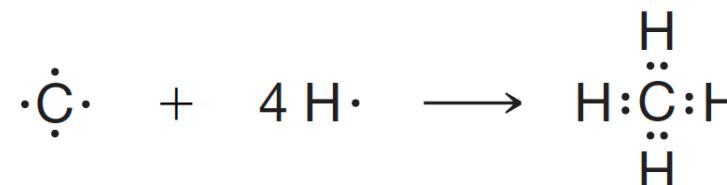
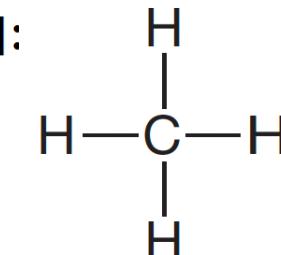
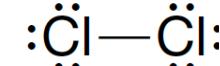
- **Covalent Bonds** are formed by sharing electrons between atoms that are similar or close in their electronegativities in order to achieve Nobel gases configurations.
- A shared electron pair between two atoms can be represented by a dash (-).
- When the atoms are identical or have equal electronegativities,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



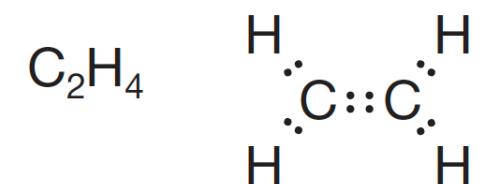
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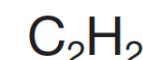
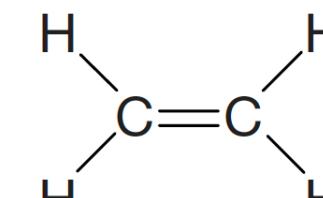
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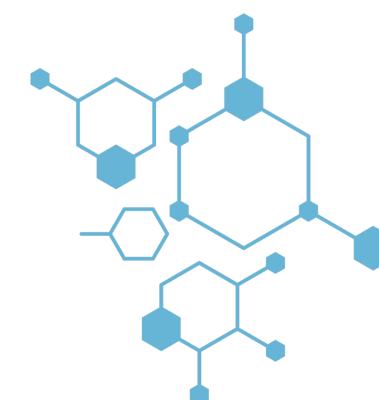
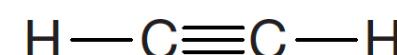
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Drawn as



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.

- 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

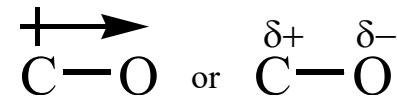


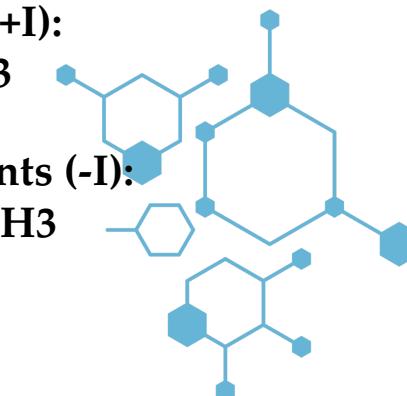
TABLE 1.1 ELECTRONEGATIVITIES OF SOME OF THE ELEMENTS

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

Increasing electronegativity

➤ Electron-donating substituents (+I):
-CH₃, -C₂H₅, -NH₂, -OH, -OCH₃

➤ Electron-withdrawing substituents (-I):
-CH₃, -C₂H₅, -NH₂, -OH, -OCH₃



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 ($\delta+$) on one atom and a partial negative charge ($\delta-$) on the other atom.
- This physical property can be measured experimentally using the following equation:

$$\mu = e \times d$$

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

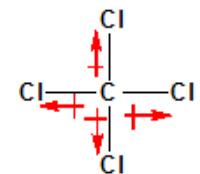
e : magnitude of separate charge (in esu)

d : distance between charges (in cm)

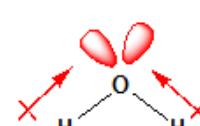
- Dipole moment of a molecule can affect other physical properties including polarity, solubility, and intermolecular forces.

TABLE 2.1 DIPOLE MOMENTS OF SOME SIMPLE MOLECULES

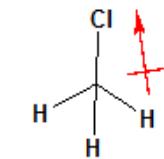
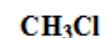
Formula	μ (D)	Formula	μ (D)
H_2	0	CH_4	0
Cl_2	0	CH_3Cl	1.87
HF	1.83	CH_2Cl_2	1.55
HCl	1.08	CHCl_3	1.02
HBr	0.80	CCl_4	0
HI	0.42	NH_3	1.47
BF_3	0	NF_3	0.24
CO_2	0	H_2O	1.85



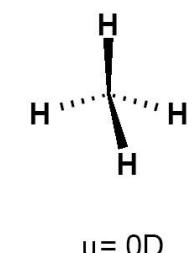
$$\mu = \text{zero}$$



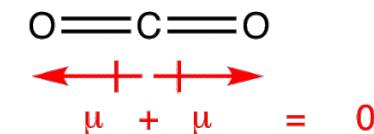
$$\mu \neq \text{zero}$$



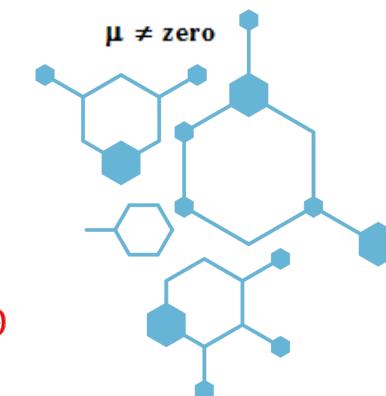
$$\mu \neq \text{zero}$$



$$\mu = 0\text{D}$$



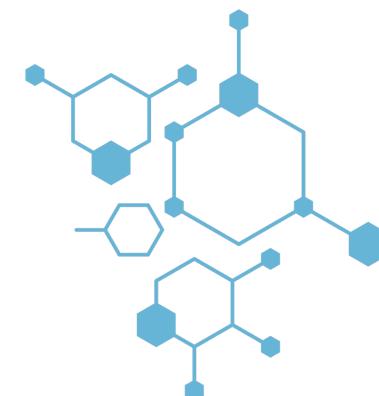
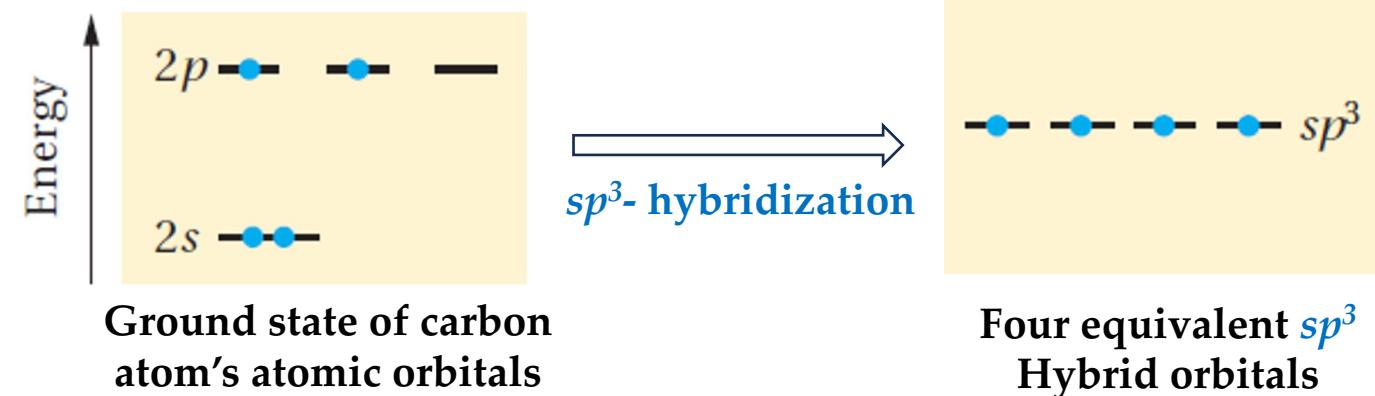
$$\mu + \mu = 0$$



4. Hybridization and Molecular Geometry

4.1 Orbitals Hybridization

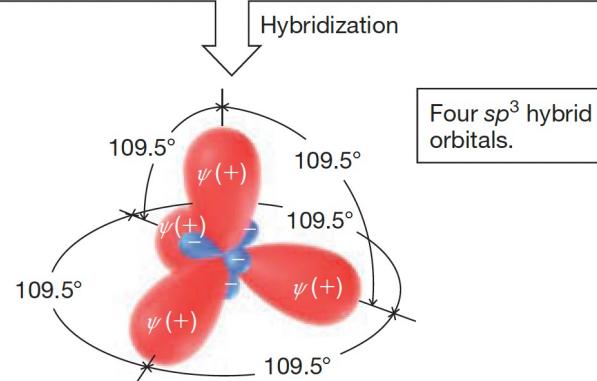
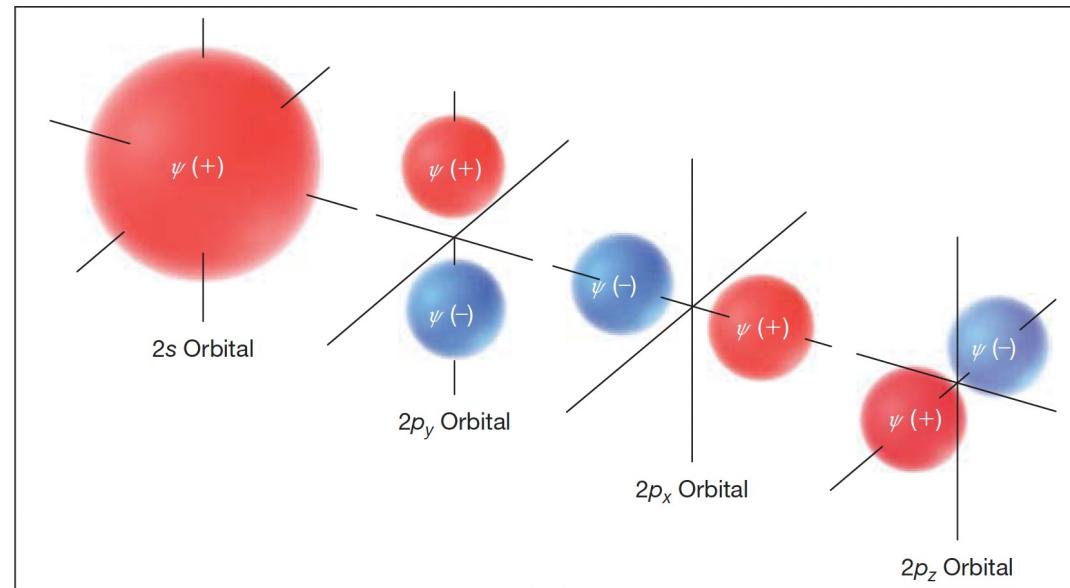
- Orbital hybridization describes how atomic orbitals mix to form new hybrid orbitals that are better suited for bonding in molecules having the same level of energy..
- It helps to explain shapes of molecules and their bond angles.
- In hydrocarbon organic molecules, there are three common types of 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 one part of s-character and three parts of p-character.



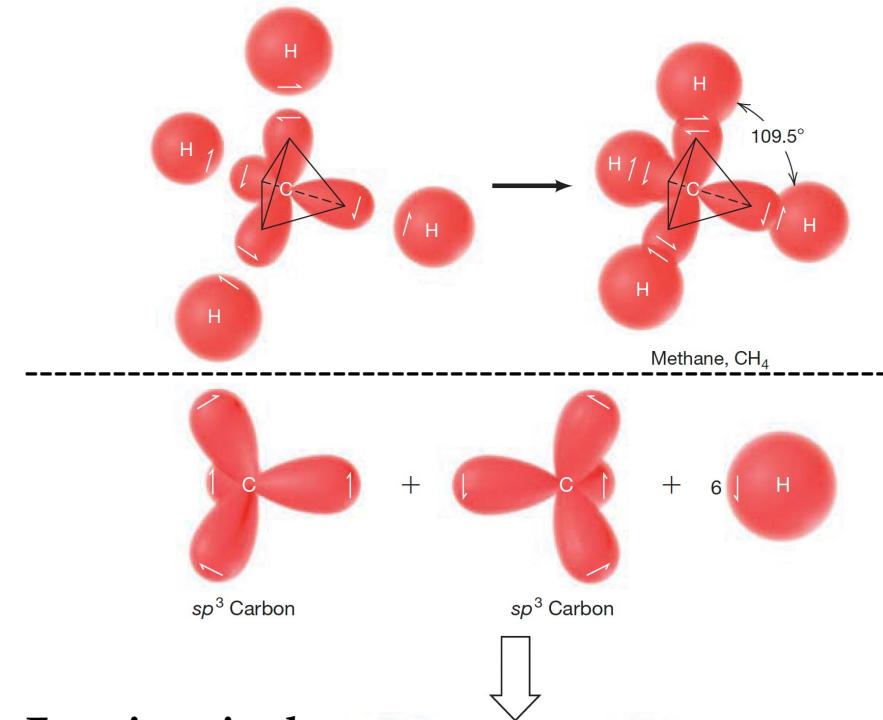
4. Hybridization and Molecular Geometry

4.1 Orbitals Hybridization

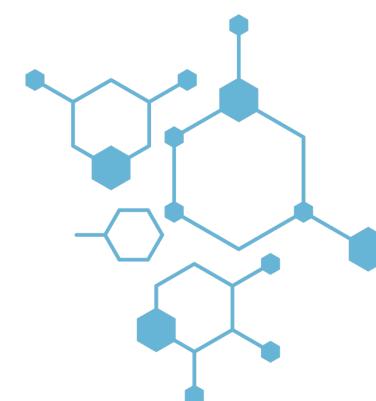
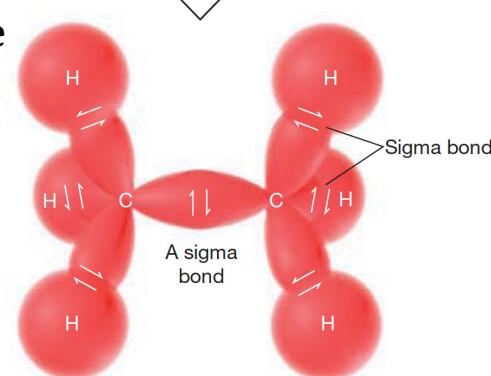
- sp^3 - Hybridization (in alkanes):



➤ Molecular Geometry of Methane (CH_4): **Tetrahedral**



➤ Forming single sigma (σ) bond in Ethane (C_2H_6)

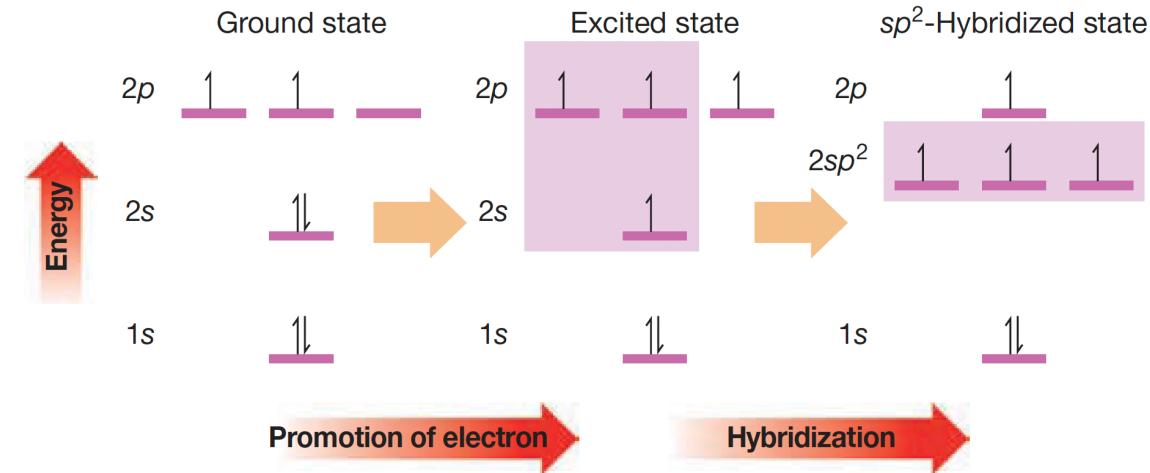


4. Hybridization and Molecular Geometry

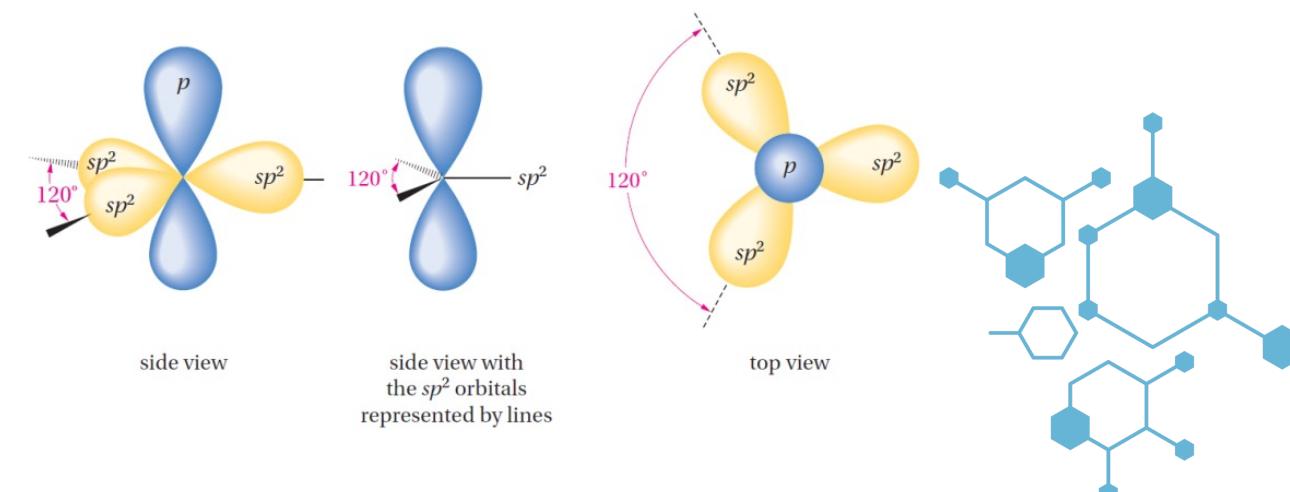
4.1 Orbitals Hybridization

- **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 $2p$ 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:

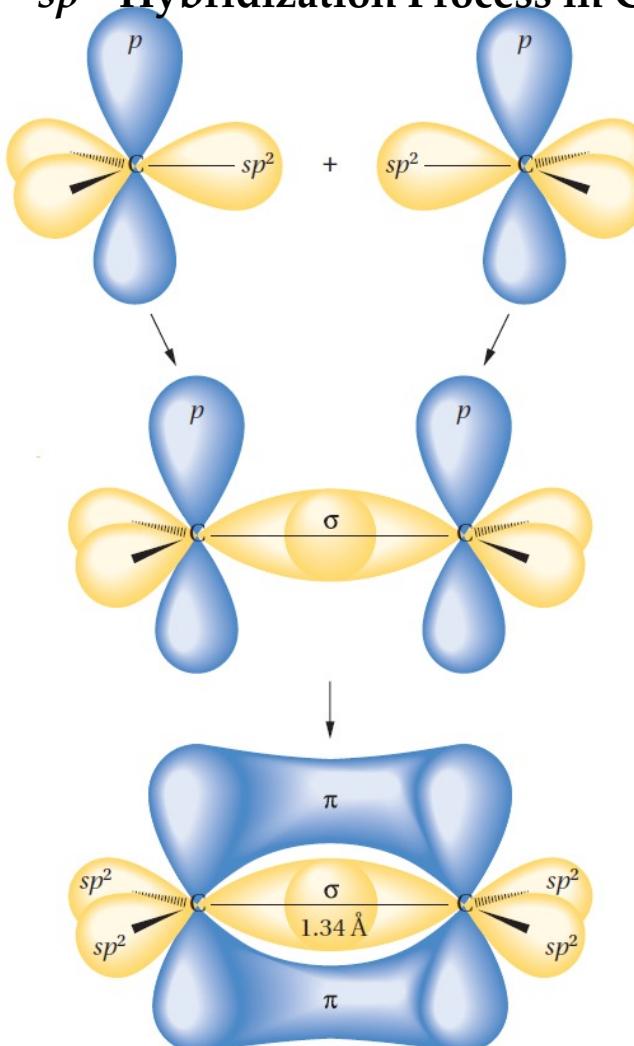


4. Hybridization and Molecular Geometry

4.1 Orbitals Hybridization

- **sp^2 - Hybridization (in alkenes)**
- **Schematic formation of a carbon–carbon double bond.** Two sp^2 carbons form a sigma (σ) bond (end-on overlap of two sp^2 orbitals) and a pi (π) 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 \AA).

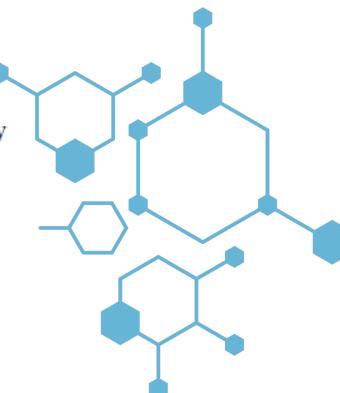
➤ sp^2 - Hybridization Process in Carbon Atom:



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

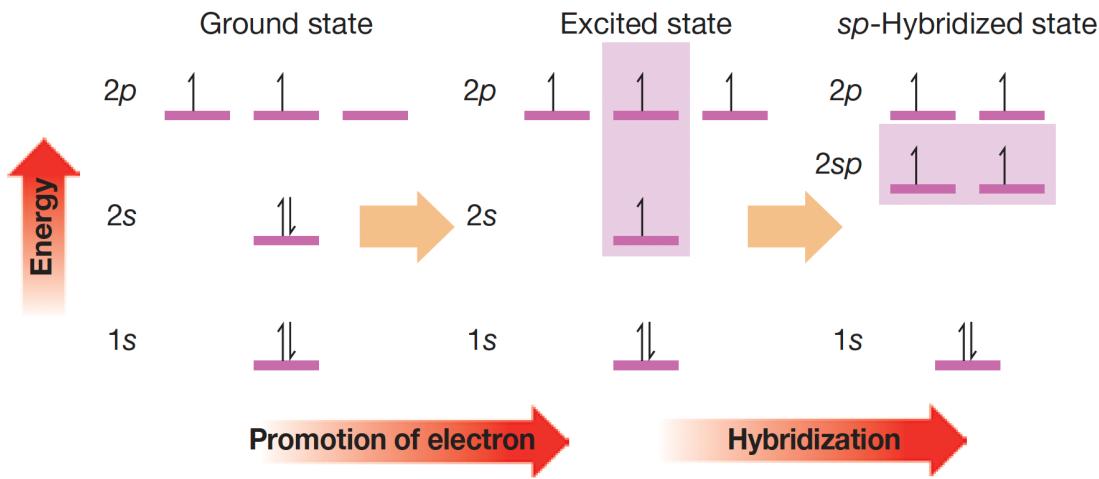


4. Hybridization and Molecular Geometry

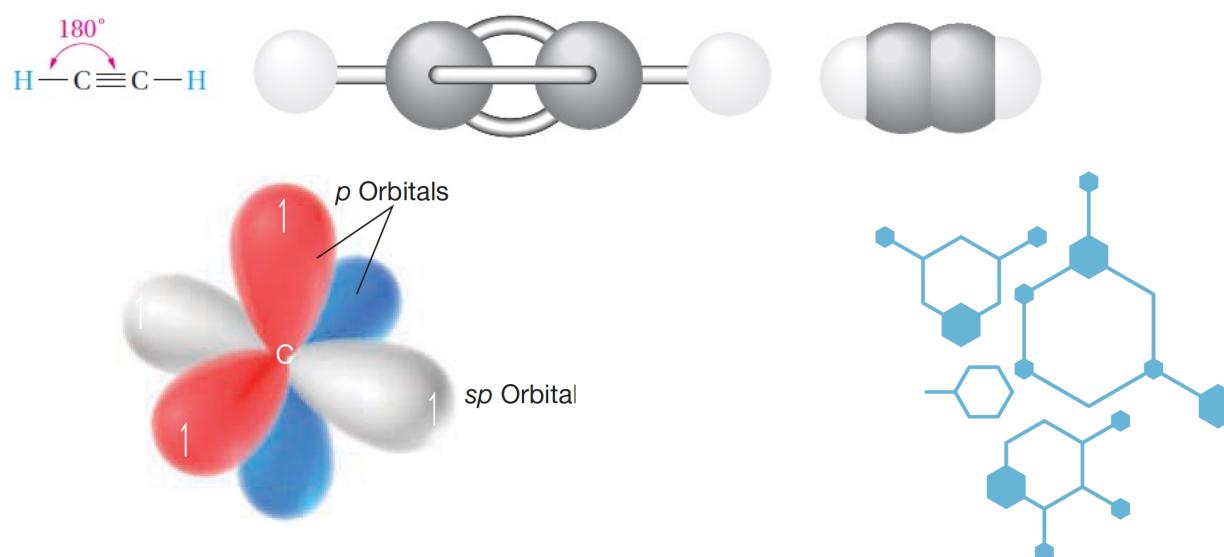
4.1 Orbitals Hybridization

- **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 *2p* 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:

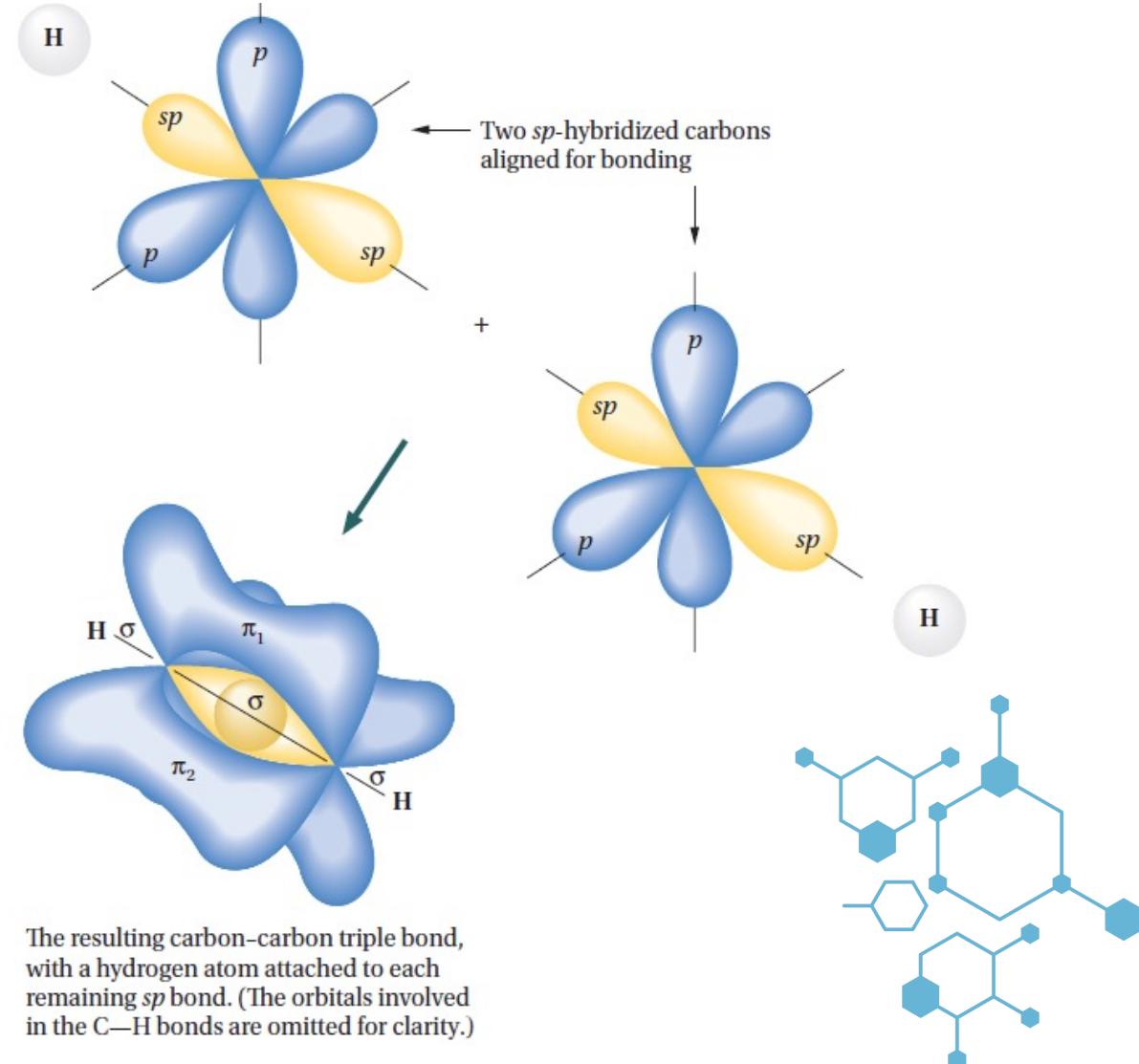


4. Hybridization and Molecular Geometry

4.1 Orbitals Hybridization

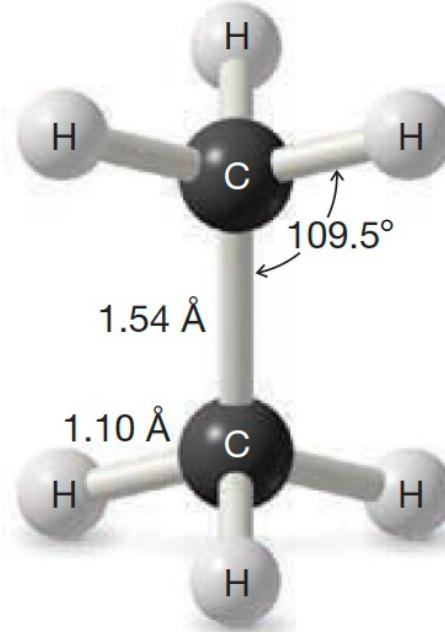
- **sp- Hybridization (in alkynes)**
- A triple bond consists of the end-on overlap of two *sp*-hybrid orbitals to form a sigma (σ) bond and the lateral overlap of two sets of parallel-oriented *p* orbitals to form two mutually perpendicular (π) bonds.
- The single sigma (σ) bond's length in unsaturated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

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

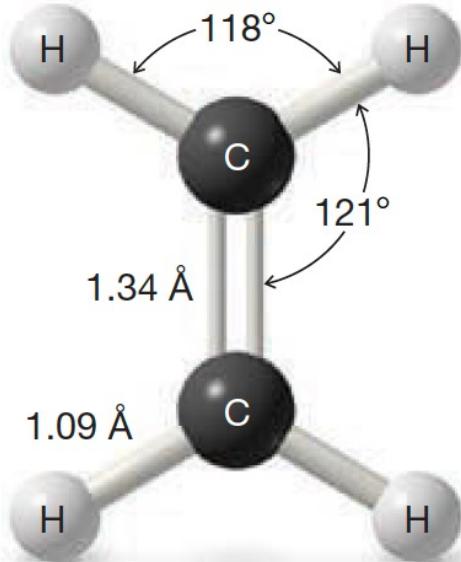


4. Hybridization and Molecular Geometry

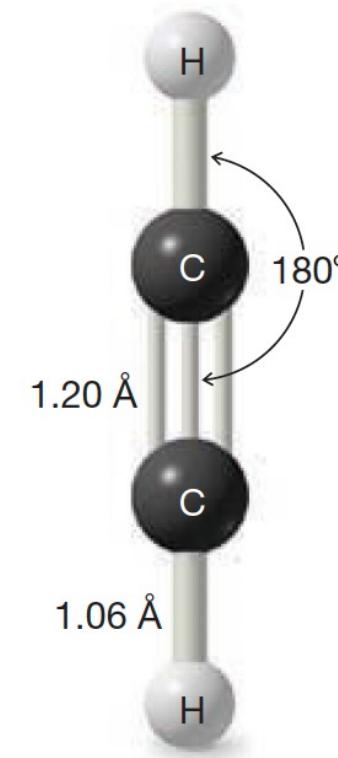
4.2 Bond Lengths – Summary Slide



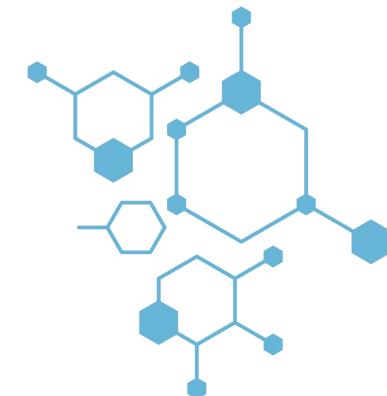
Molecule name: Ethane (Alkane)
Hybridization type: sp^3
Bond type: single sigma (σ) bond
Molecular geometry: Tetrahedral
Bond Angle: 109.5°
Bond Length: 1.54 Å



Molecule name: Ethene (Alkene)
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 Å



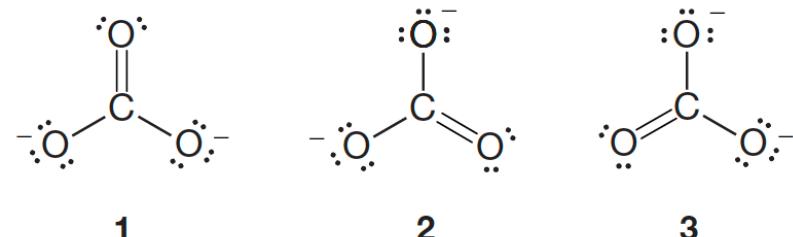
Molecule name: Ethyne (Alkyne)
Hybridization type: sp
Bond type: single sigma (σ) bond and two double (π)
Molecular geometry: Linear
Bond Angle: 180°
Bond Length: 1.20 Å



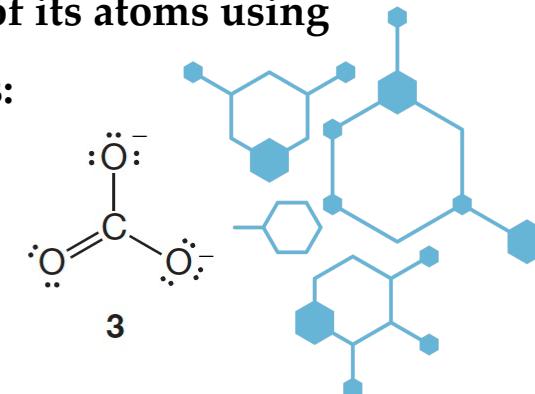
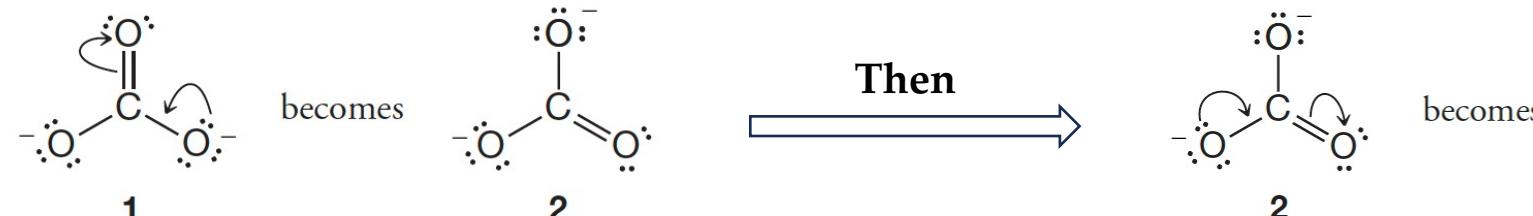
5. Resonance and Delocalization

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:



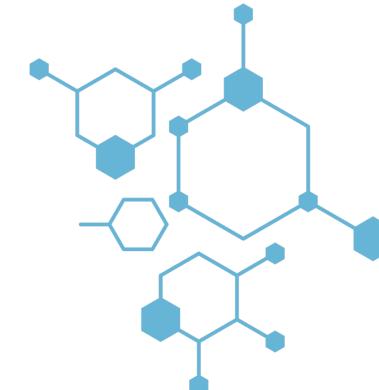
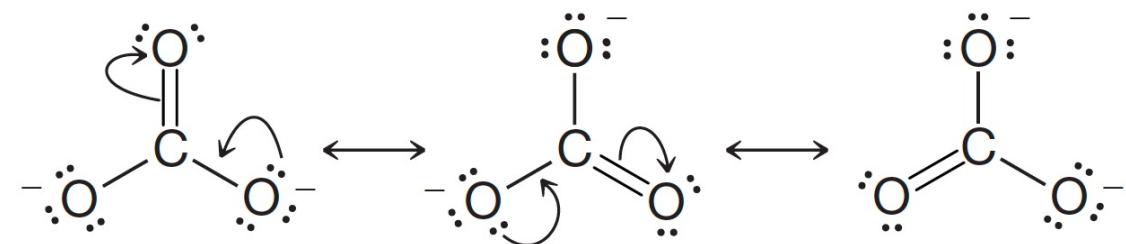
- The resonance structures of carbonate ion can be presented be delocalizing the electron pair of its atoms using The curved arrows, which emphasizes to move the electron pairs NOT the re-position its atoms:



5. Resonance and Delocalization

5.2 The Use of Curved Arrows

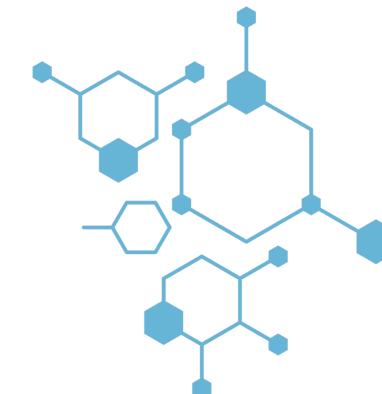
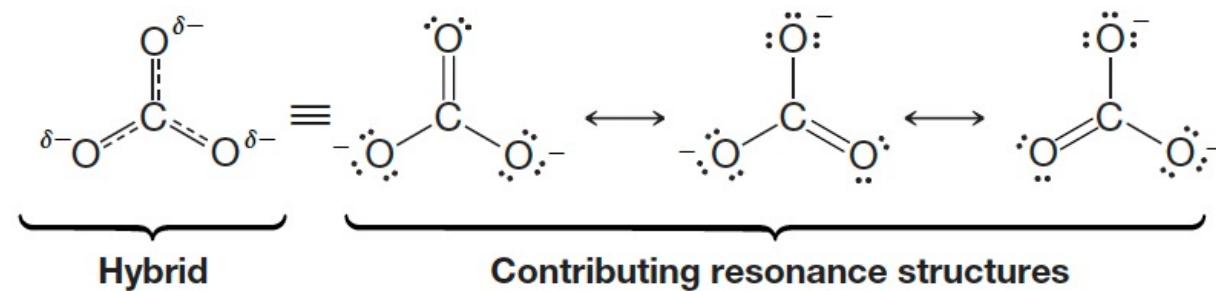
- In organic chemistry, curved arrows (\curvearrowright) are used to draw resonance structures as well as to illustrate reaction mechanisms.
- Important notes on the proper use of the curved arrows:
 - Curved arrows show the movement of both bonding and unshared electrons on atoms.
 - Each curved arrow 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

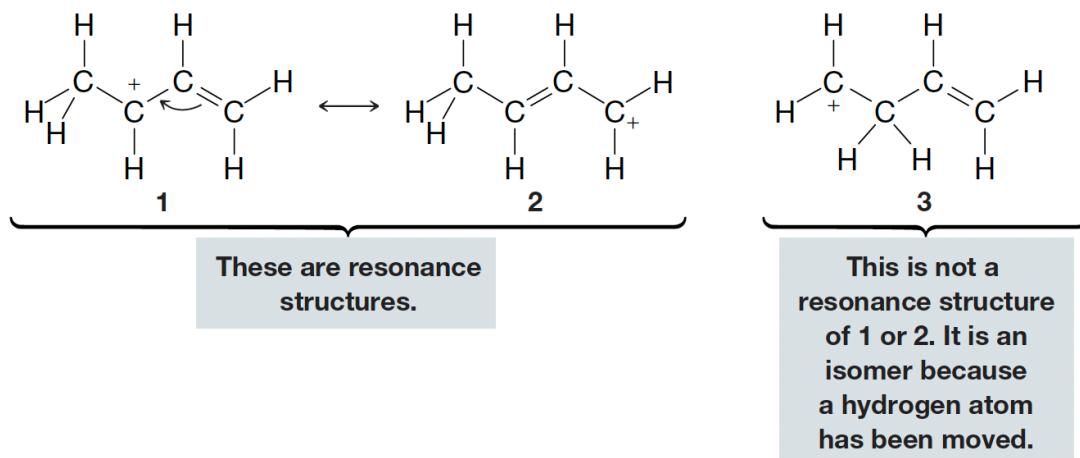
- A **Hybrid Structure** is defined as the actual electronic structure of a molecule that has more than one valid resonance structures.
- Electrons are delocalized across atoms rather than fixed in one bond or position.
- The solid and dashed lines in the hybrid structure indicates the alternation between 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.



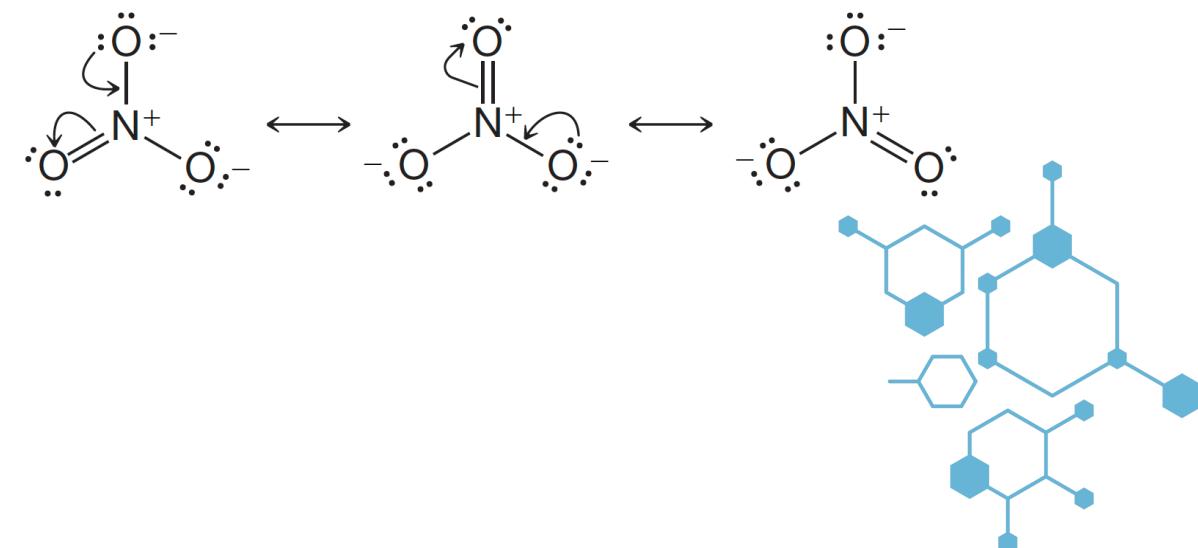
5. Resonance and Delocalization

5.4 Rules for Writing Resonance Structures

- 1) Resonance structures do not exist in real reaction flow. The real molecule or ion is a hybrid of all of its resonance structures.
- 2) Bonding electrons or unshared electron pairs are only allowed to delocalize across a molecule or ion through its atoms.
- 3) All resonance structures must be drawn properly as Lewis structures.
- 4) The energy of the hybrid structure is lower than the energy of any contributing structures.



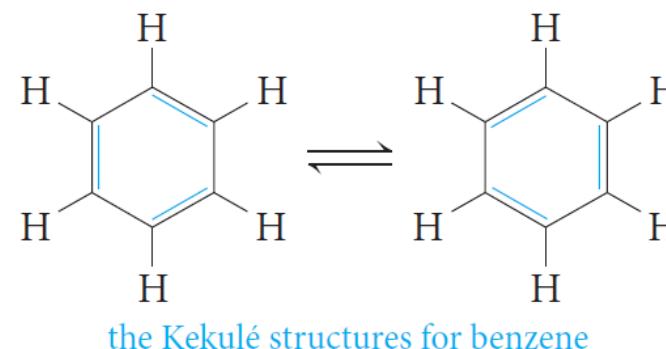
➤ Another example of resonance structure for nitrate ion (NO_3^-):



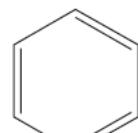
5. Resonance and Delocalization

5.5 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.
- Kekulé 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 double bonds.



the Kekulé structures for benzene

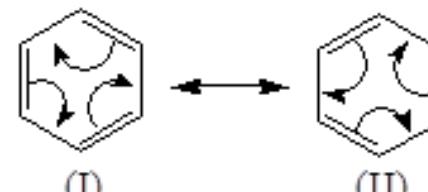


Kekulé

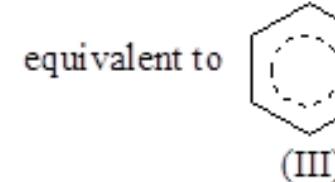


delocalized pi cloud

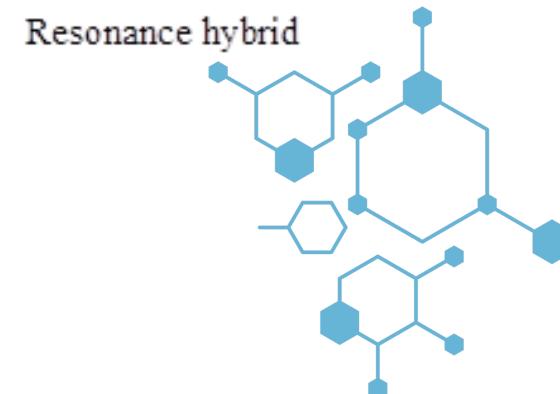
➤ Resonance Model for Benzene:



Contributing structures



equivalent to



Resonance hybrid