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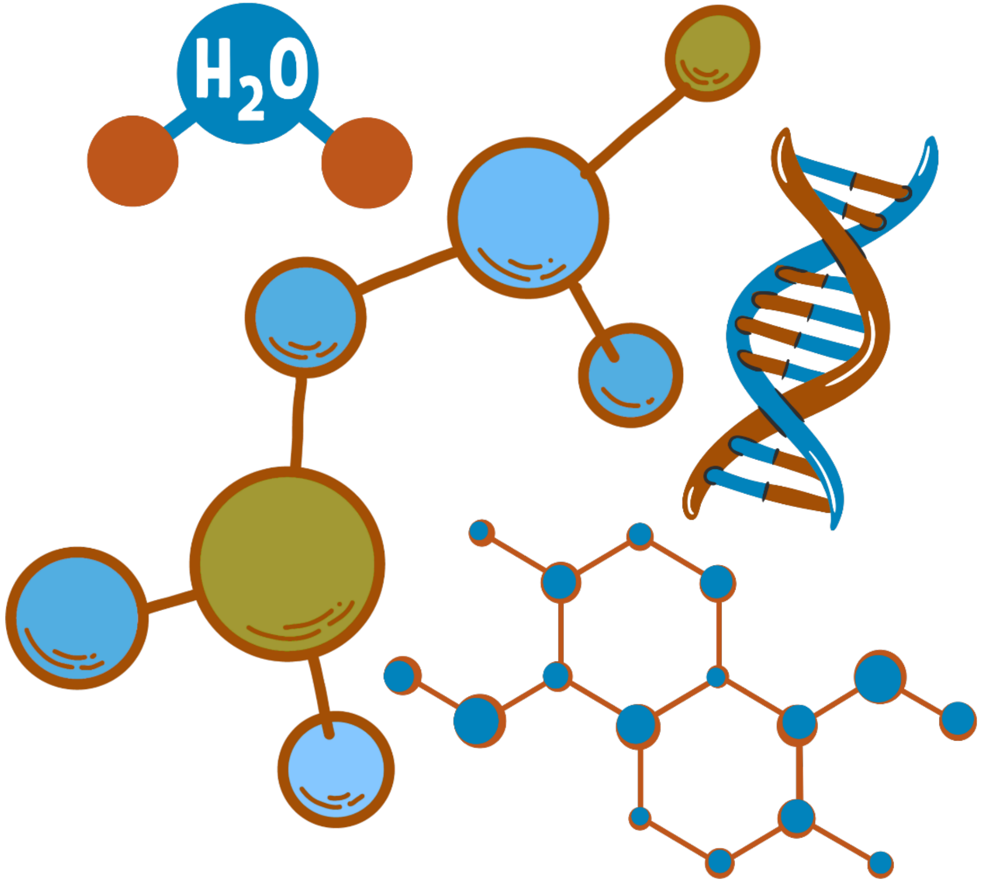
Chapter 1:
Introduction to Organic Chemistry



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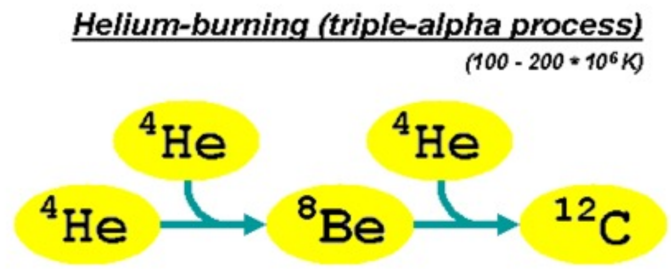
1. Origins and Scope of Organic Chemistry

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.
- **The modern definition of *Organic Chemistry:***
  - It is the study of carbon/hydrogen-based compounds and their corresponding derivatives.



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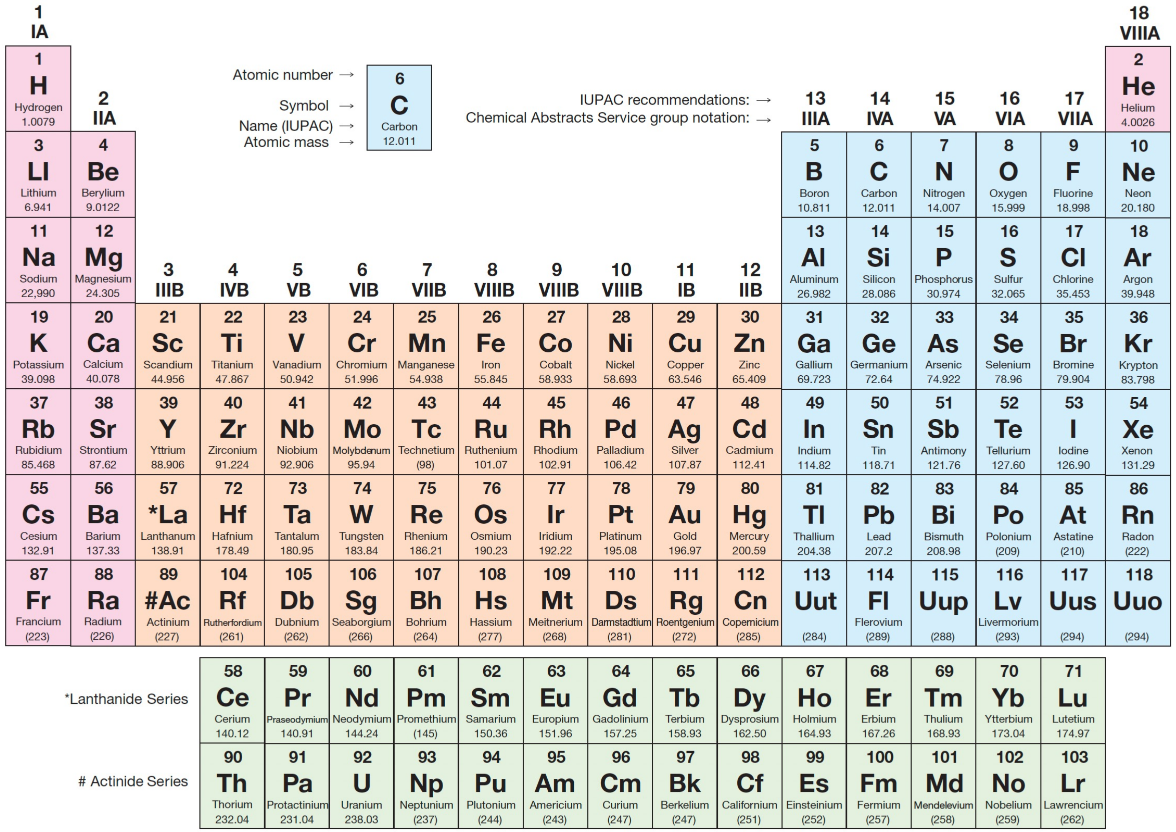
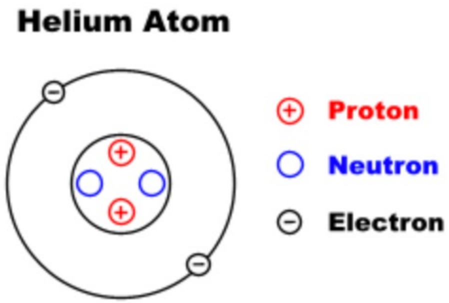
2. Atomic structure, Electron Configuration, and Molecular Orbitals

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.





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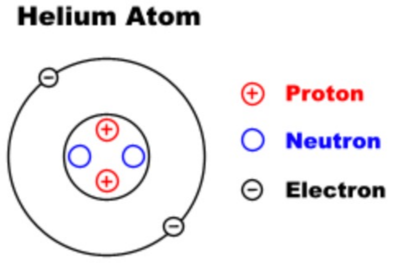
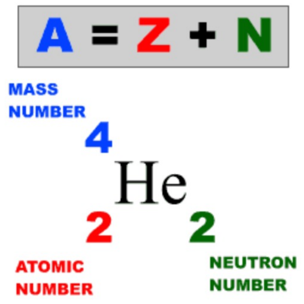
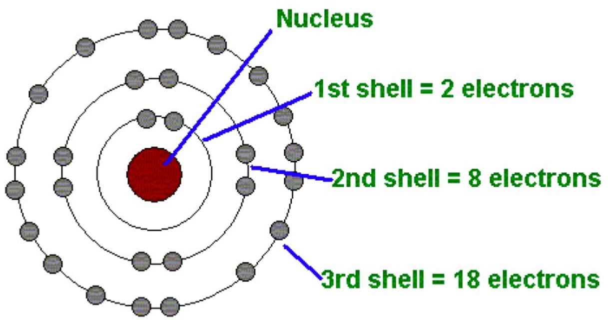
2. Atomic structure, Electron Configuration, and Molecular Orbitals

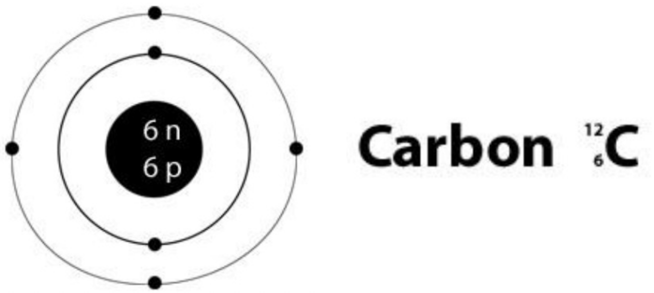
2.1 Atomic Structure

- 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
Atomic mass → 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
1 H Hydrogen 1.0079																	2 He Helium 4.0026
3 Li Lithium 6.941	4 Be Berylium 9.0122											5 B Boron 10.811	6 C Carbon 12.011	7 N Nitrogen 14.007	8 O Oxygen 15.999	9 F Fluorine 18.998	10 Ne Neon 20.180
11 Na Sodium 22,990	12 Mg Magnesium 24.305											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 Ar Argon 39.948
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)
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)	110 Ds Darmstadtium (281)	111 Rg Roentgenium (272)	112 Cn Copernicium (285)	113 Uut (284)	114 Fl Flerovium (289)	115 Uup (288)	116 Lv Livermorium (293)	117 Uus (294)	118 Uuo (294)

*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	64 Gd Gadolinium 157.25	65 Tb Terbium 158.93	66 Dy Dysprosium 162.50	67 Ho Holmium 164.93	68 Er Erbium 167.26	69 Tm Thulium 168.93	70 Yb Ytterbium 173.04	71 Lu Lutetium 174.97
# 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)	96 Cm Curium (247)	97 Bk Berkelium (247)	98 Cf Californium (251)	99 Es Einsteinium (252)	100 Fm Fermium (257)	101 Md Mendelevium (258)	102 No Nobelium (259)	103 Lr Lawrencium (262)

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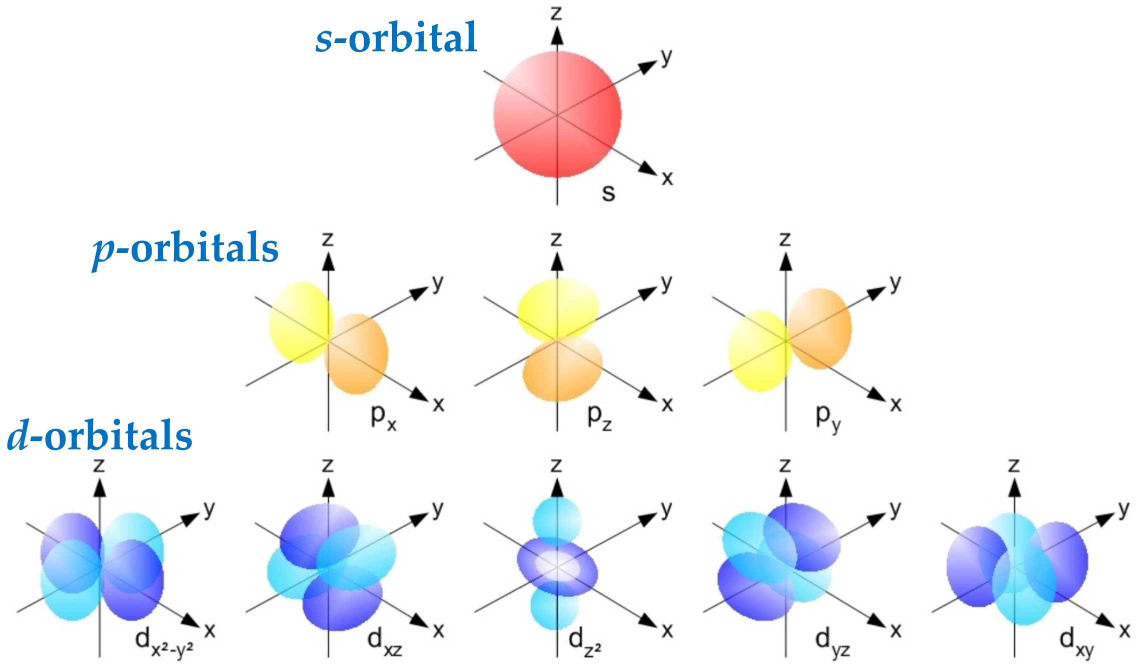
2. Atomic structure, Electron Configuration, and Molecular Orbitals

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.



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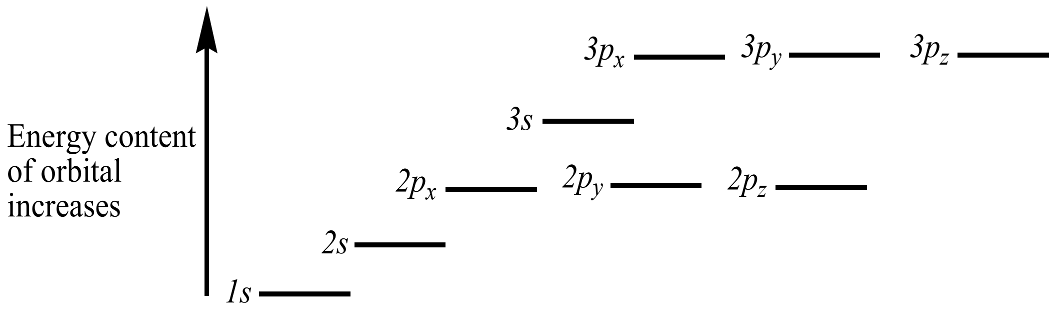
2. Atomic structure, Electron Configuration, and Molecular Orbitals

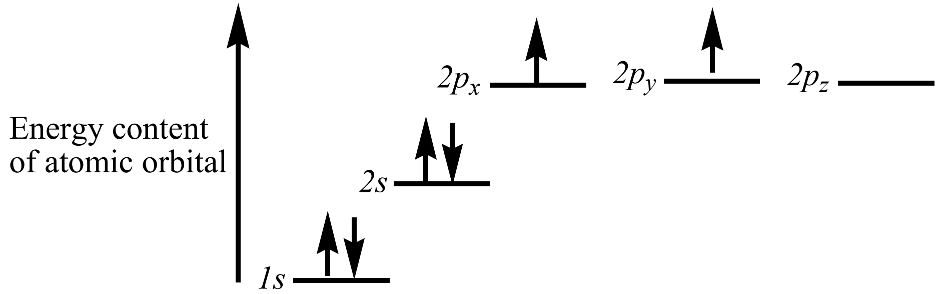
2.2 Atomic orbitals and electron configuration

- **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):**

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



Energy level diagram for carbon.

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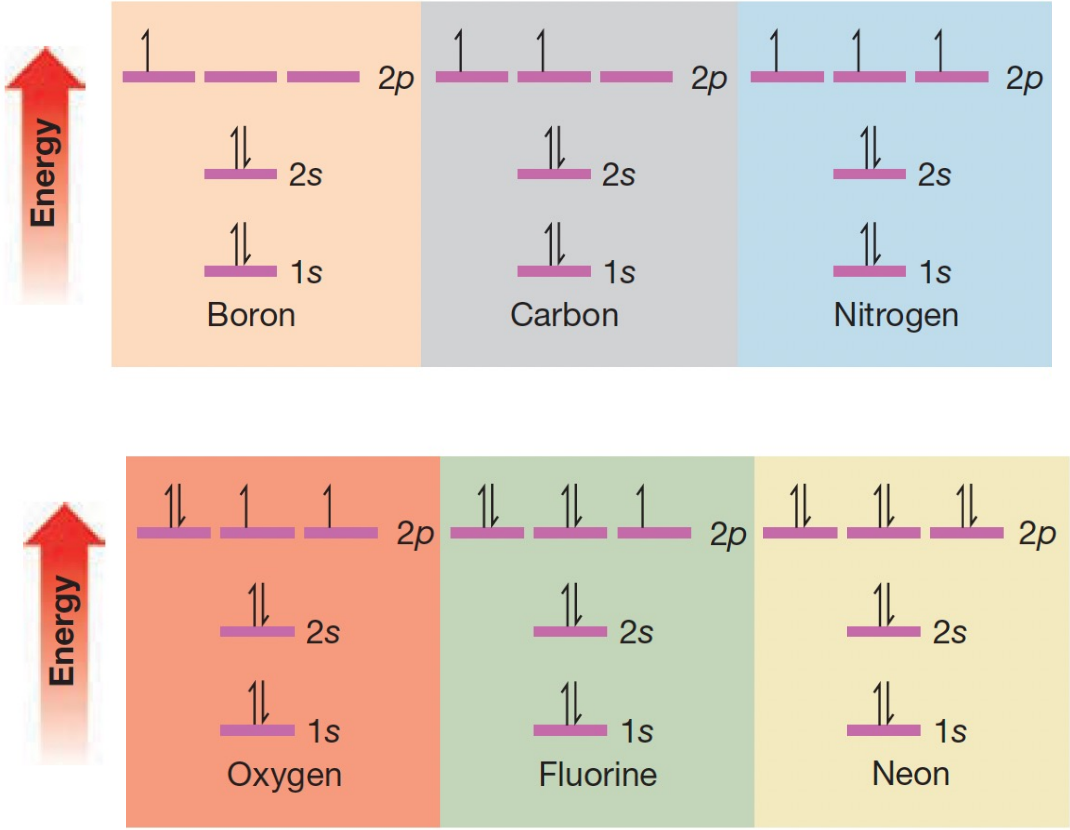
2. Atomic structure, Electron Configuration, and Molecular Orbitals

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.**



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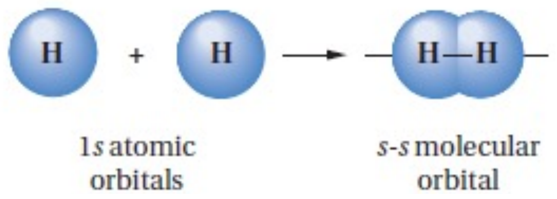
2. Atomic structure, Electron Configuration, and Molecular Orbitals

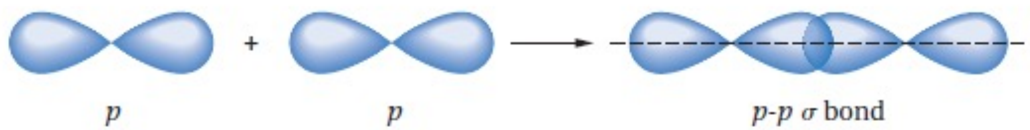
2.3 Molecular Orbitals (MOs)

- 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:

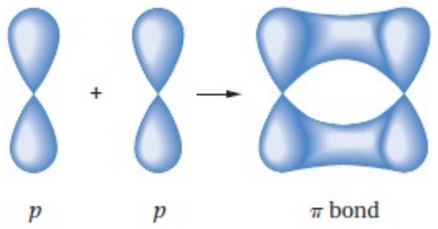


➢ Two (*p*) atomic orbitals overlap to form (*σ* bond):



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

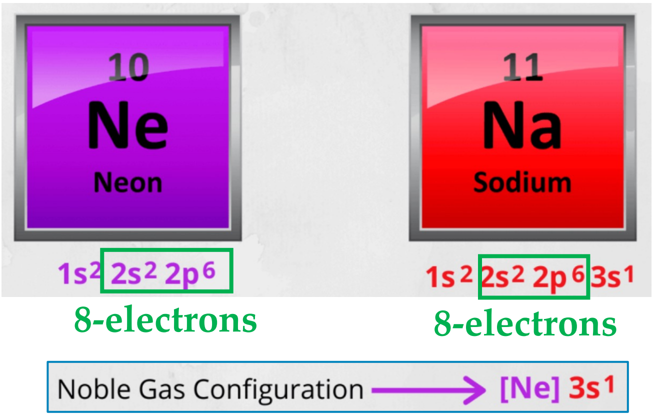
➢ Two (*p*) atomic orbitals overlap to form (*π* bond):



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.**



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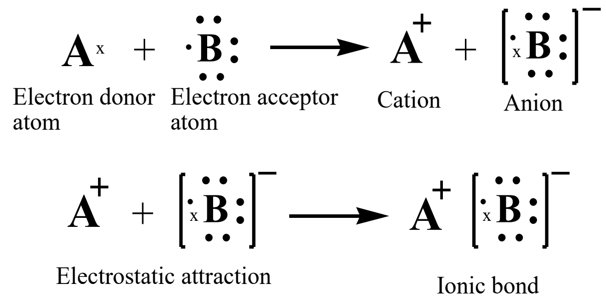
3. Chemical Bonding

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*).**



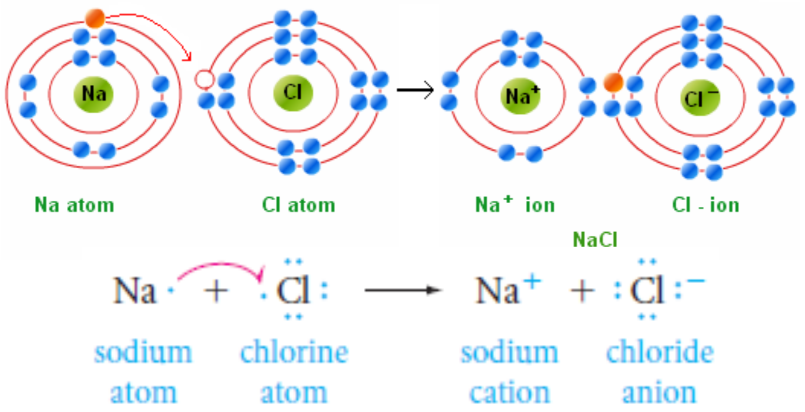


TABLE 1.1 ELECTRONEGATIVITIES OF SOME OF THE ELEMENTS

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

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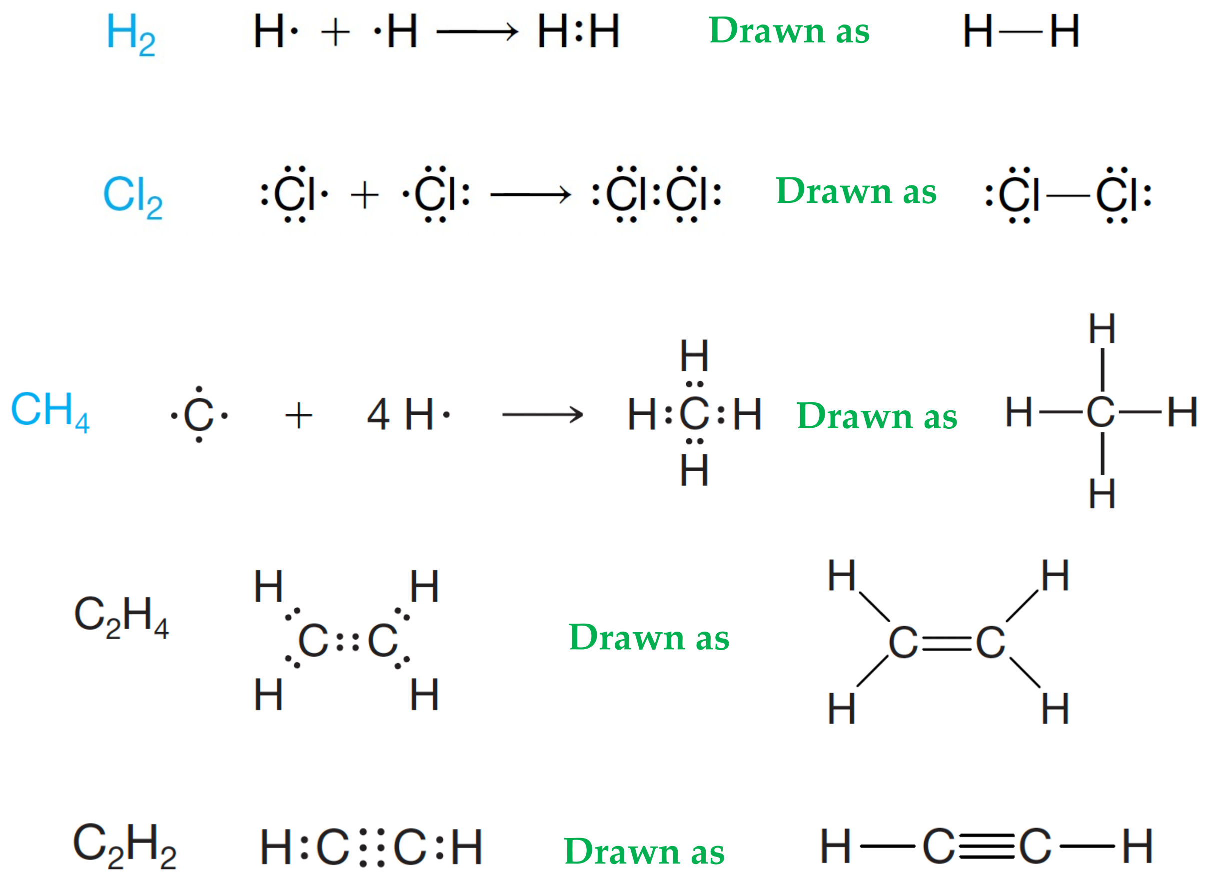
3. Chemical Bonding

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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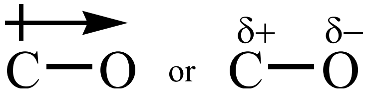
3. Chemical Bonding

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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↑ Increasing electronegativity

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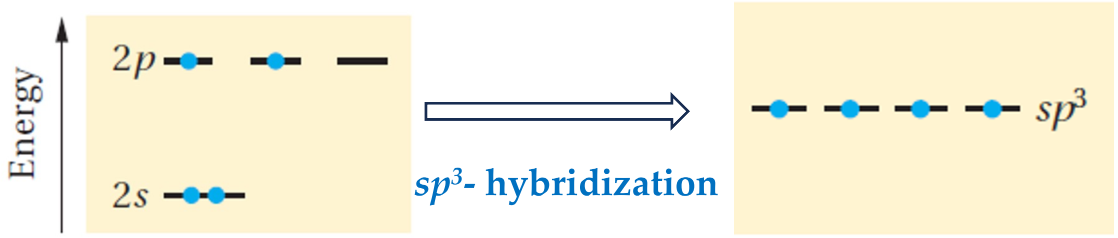
4. Hybridization and Molecular Geometry

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.



Ground state of carbon atom's atomic orbitals

Four equivalent *sp^3* Hybrid orbitals

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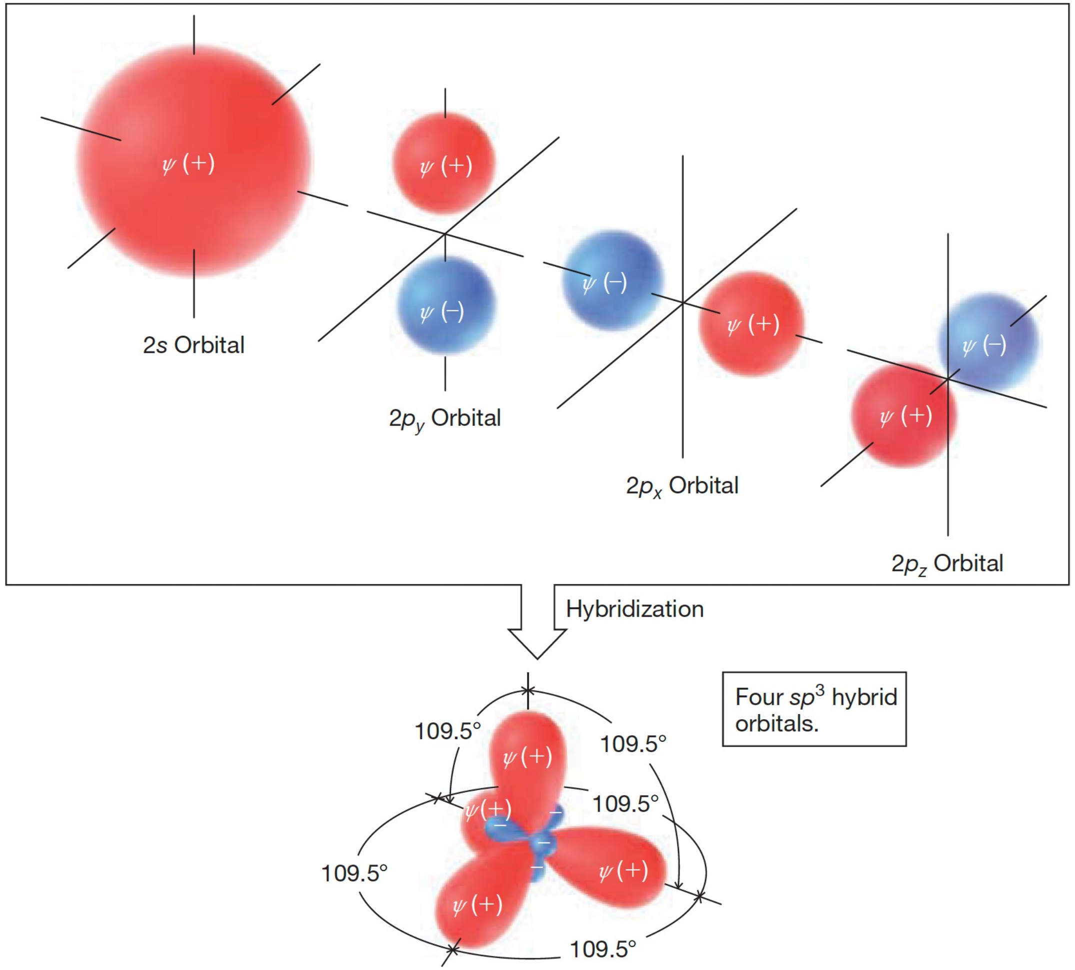
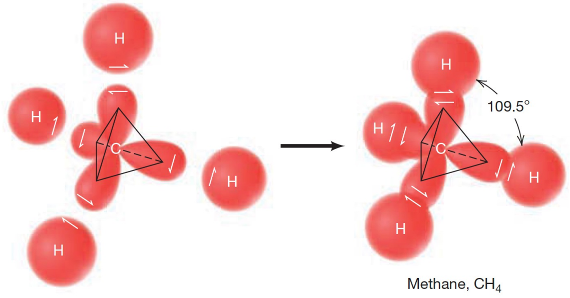
4. Hybridization and Molecular Geometry

4.1 Orbitals Hybridization

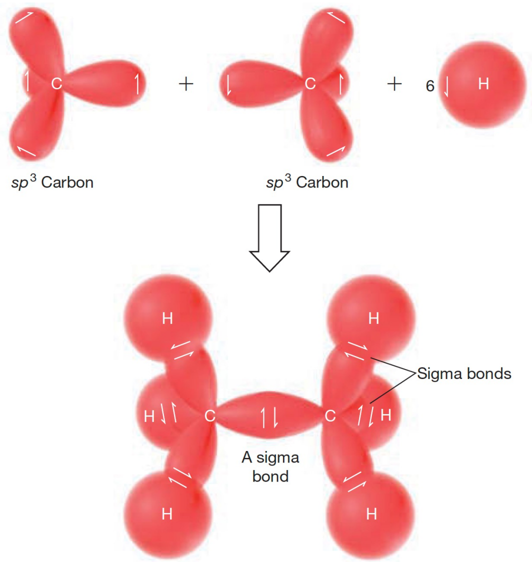
- *sp^3*- Hybridization (in alkanes):



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



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



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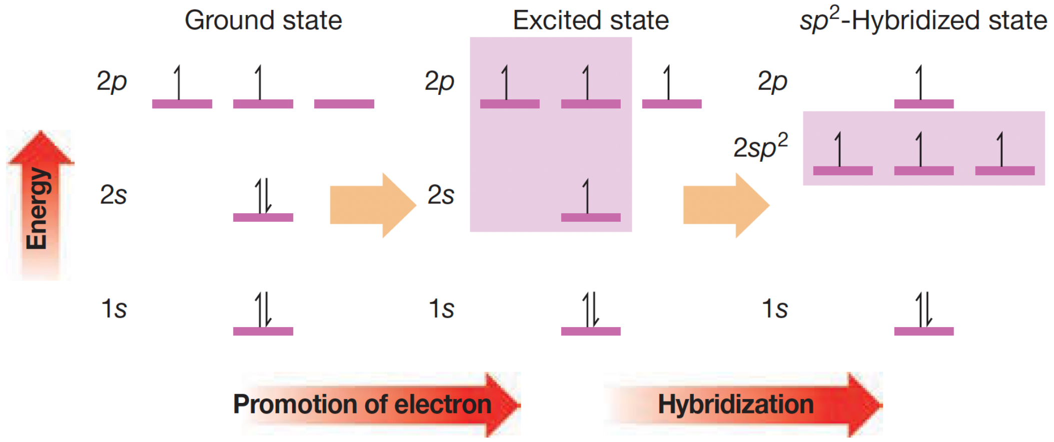
4. Hybridization and Molecular Geometry

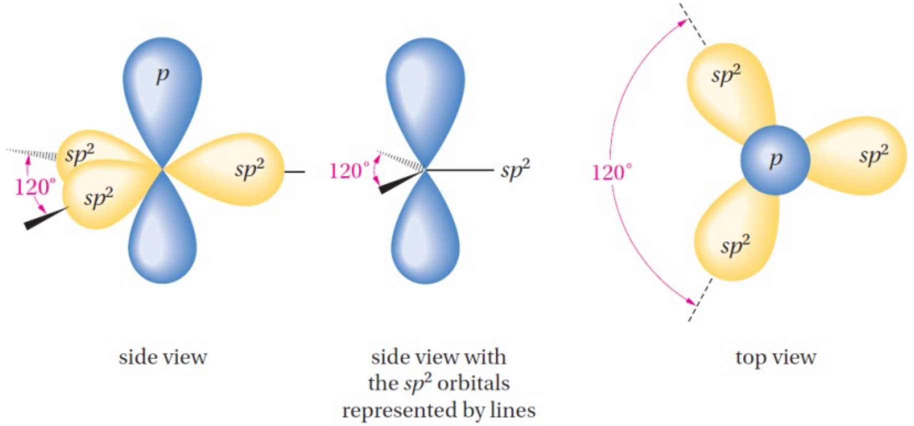
4.1 Orbitals Hybridization

- *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:



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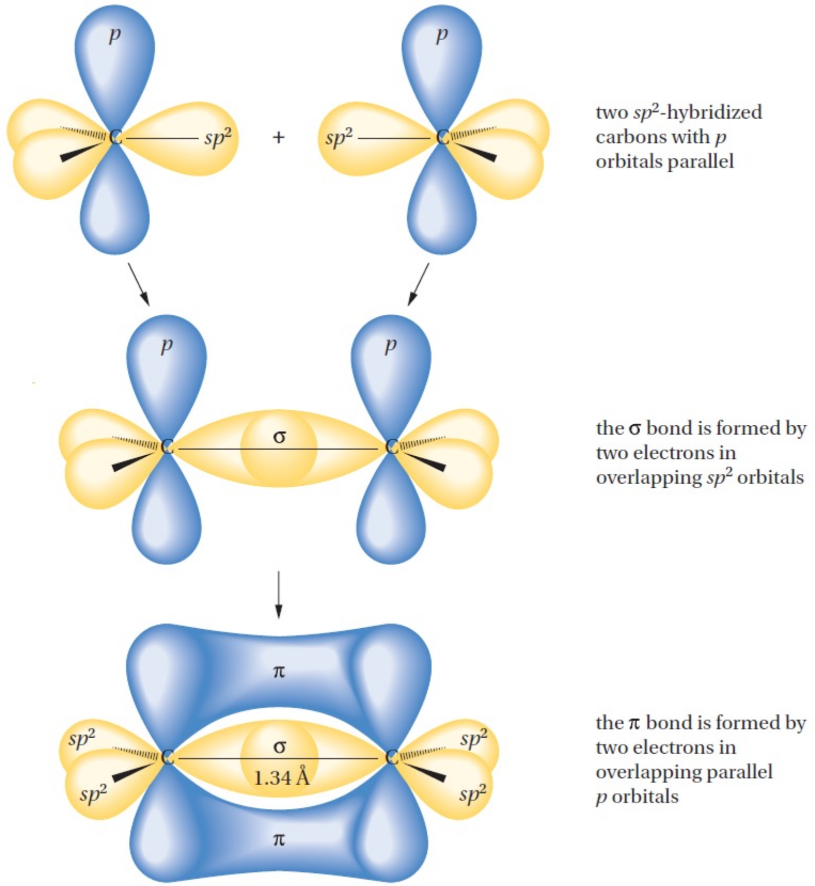
4. Hybridization and Molecular Geometry

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:



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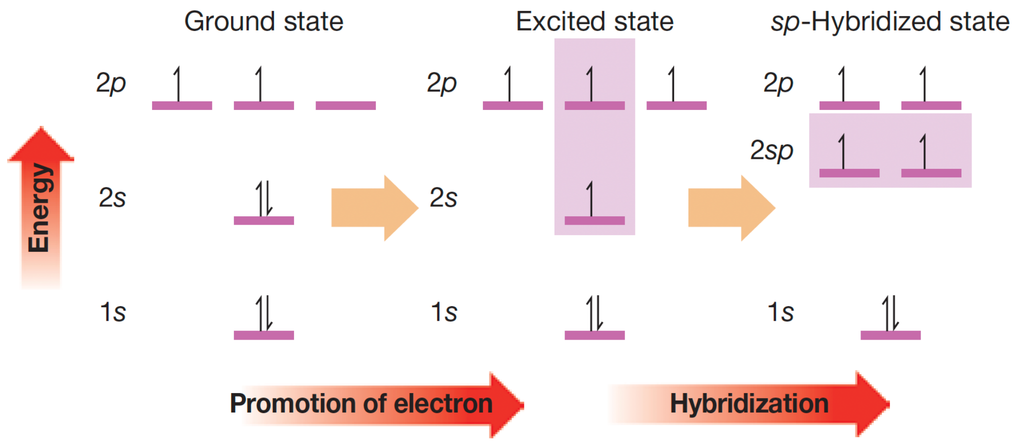
4. Hybridization and Molecular Geometry

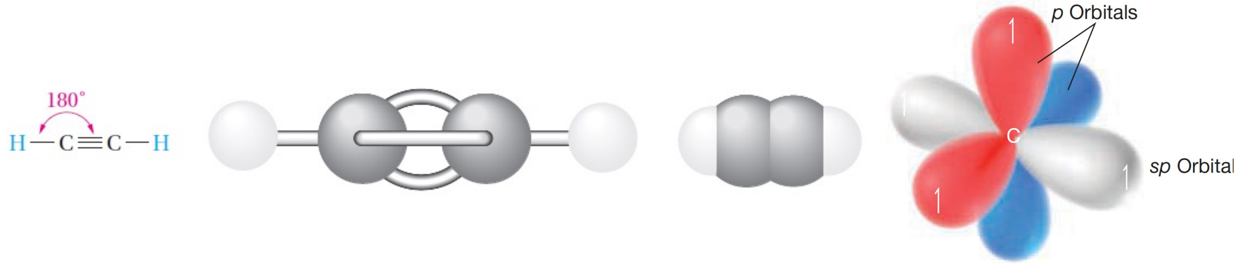
4.1 Orbitals Hybridization

- *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:



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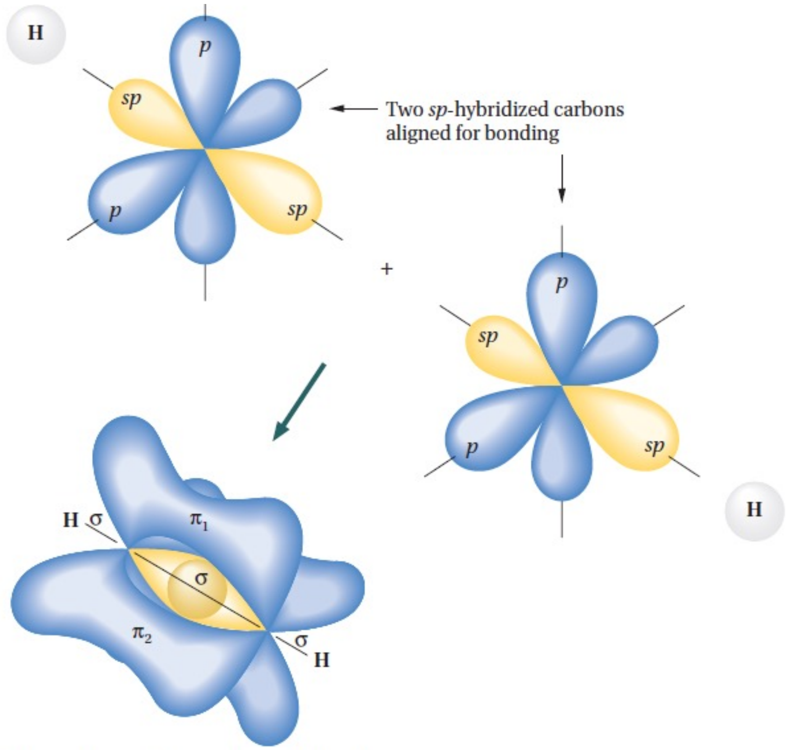
4. Hybridization and Molecular Geometry

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:**



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.)

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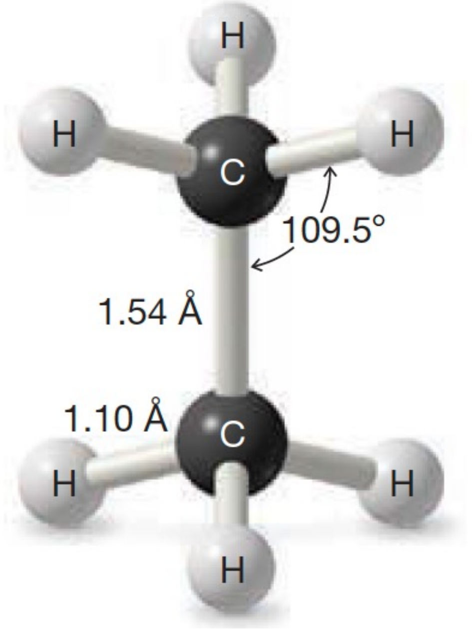
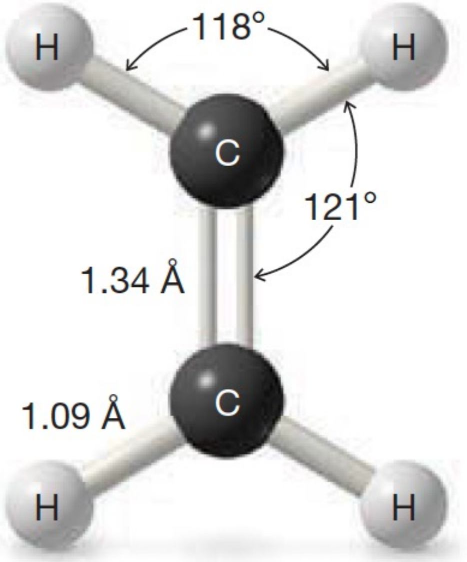
4. Hybridization and Molecular Geometry

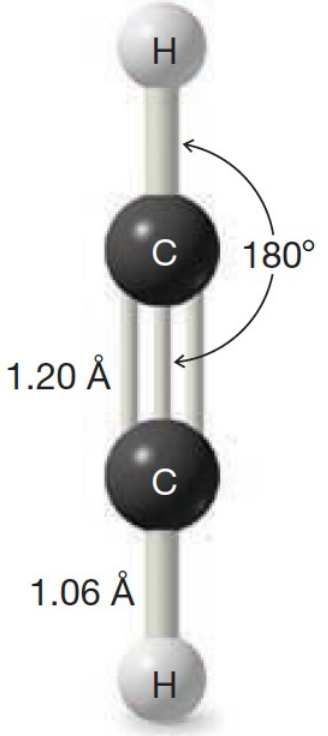
4.2 Summary Slide



- **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