Atomic Structure
Introduction:

An atom consists of a nucleus composed of protons and neutrons and electrons which encircle the nucleus.

- Protons and electrons have same and opposite charge of 1.6 x 10^{-19} C.
- Atomic number (Z) = Number protons = number of electrons.
- Atomic mass (A) = proton mass + neutron mass.
- Isotopes are the same element having different atomic masses. Number of protons in isotopes remains same while number of neutrons varies.
- Atomic mass unit (amu) = 1/12 mass of Carbon 12 (12C)
- 1 mol of substance contains 6.023 x 10^{23} (Avogadro's number) atoms or molecules.
- Atomic weight = 1 amu/atom (or molecule) = 1 g/mol = Wt. of 6.023 x 10^{23} atoms or molecules

For example, atomic weight of copper is 63.54 amu/atom or 63.54 g/mole

• Materials → Molecules → Atoms
• Atoms = protons (p) + neutrons (n) + electrons (e)
• Protons and neutrons are made of quarks

Nonlocalized behavior of electrons in metals

• High electrical conductivity
 - electrons move easily when E-field applied
• High thermal conductivity
 - the electrons can carry energy through metal
• High density
 - outer shell removed from atoms, so can be packed together
• High ductility
 - if metal distorted, bent, electrons can quickly move to compensate
 - metal bond is not directional

Quantum numbers

Four parameters or numbers called Quantum numbers are needed to describe the distribution and position of electrons in an atom.
The first three of them (n, l, ml) describe the size, shape, and spatial orientation of the probability density distribution of electrons .

Principal quantum number, n

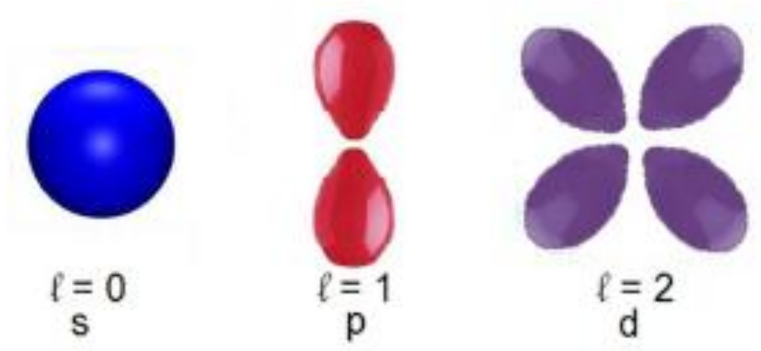
It describes electron shells as shown in the Bohr model.
Values of n can be 1, 2, 3, 4 … corresponding to electron shells K, L, M, N …..
The value of ***n*** also determines the size or distance of the shells from the nucleus.

Azimuthal or Angular quantum number, l

It signifies subshell or electron orbital – s, p, d, f and so on.

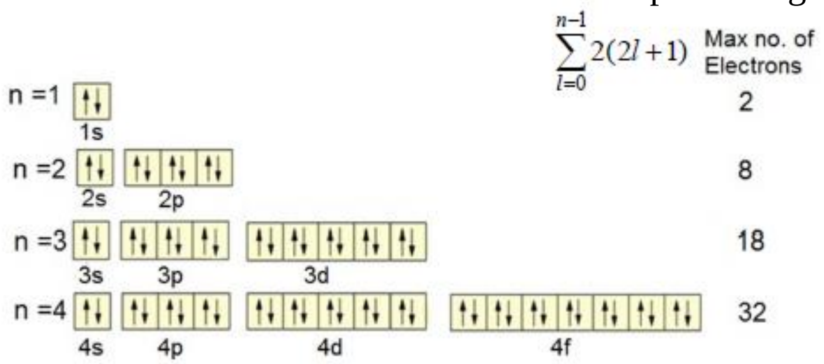
, *l* can take values of from 0 to n-1. K shell, n = 1, one s orbital. L , n =2, two orbitals, s, p. M, n =3, three orbitals s, p, d. N, n =4, four orbitals s, p, d, f and so on.

The value of l decides the shape of the orbital as shown in the figure below. s orbital (***l*** = 0) – spherical, p (***l*** = 1) – polar or dumbbell shaped, d (***l*** =2) – double-dumbbell shaped



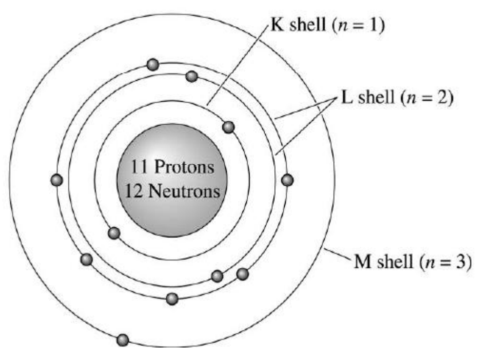
Electron Configuration

The quantum mechanic principles as discussed before allow determination of electron configuration i.e. the manner in which electron states are occupied in a given atom.



Electron configuration based on quantum numbers. Total number of electrons in a shell is $2n^2$ or $\sum_{l=0}^{n-1} 2(2l+1)$

e.g.The atomic structure of sodium, atomic number 11, showing the electrons in the K, L, and M quantum shells



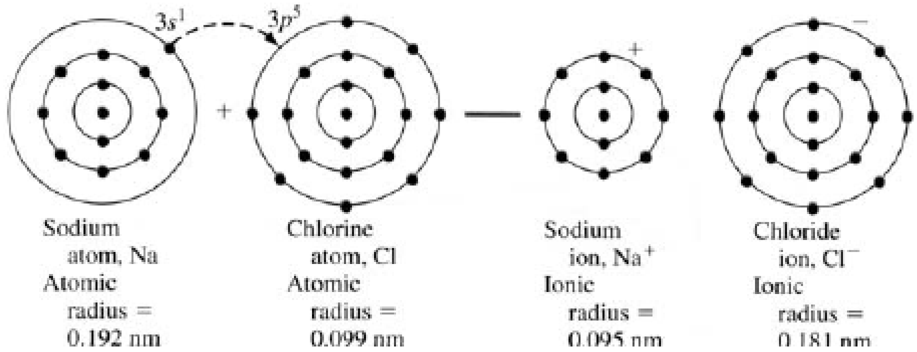
Types of atomic and molecular bonds

• ***Primary atomic bonds***

1. Ionic (large interatomic forces, nondirectional, electron transfer, coulombic forces) Typically between highly electropositive (metallic) and electronegative (nonmetallic) elements

NaCl Na $1s^2 2s^2 p^6 3s$ Cl $1s^2 2s^2 p^6 3s^2 p^5$

Na^+ $1s^2 2s^2 p^6$ Cl^- $1s^2 2s^2 p^6 3s^2 p^6$



2. Covalent (large interatomic forces, localized (directional), electron sharing)

•Takes place between elements with small difference in electronegativity

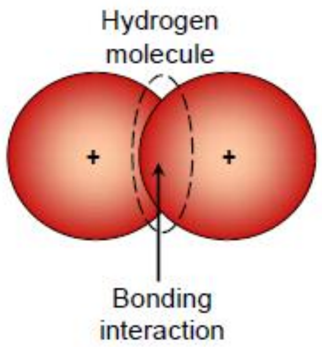
- F, O, N, Cl, H, C, Si…

• *s* and *p* electrons are commonly shared to attain noble gas electron configuration

• Multiple bonds can be formed by one atom

Hydrogen molecule 2 H: 1s → H_2 $1s_2$

H· + H· →H : H (electron –pair covalent bond)



Carbon-containing molecules

• C and H: hydrocarbons

• Structural formulas: CH_4 (methane), C_2H_6 (ethane), and C_4H_{10} (normal butane)

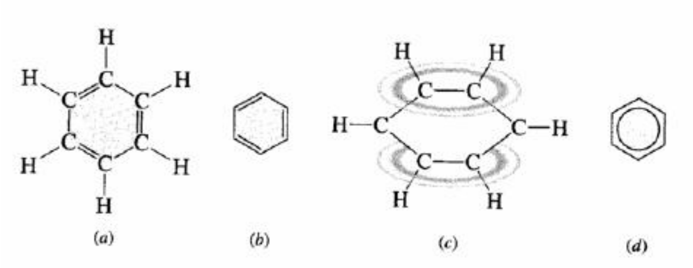
• Saturated C_nH_{2n+2}

- strong bonds inside molecule, weak between molecules

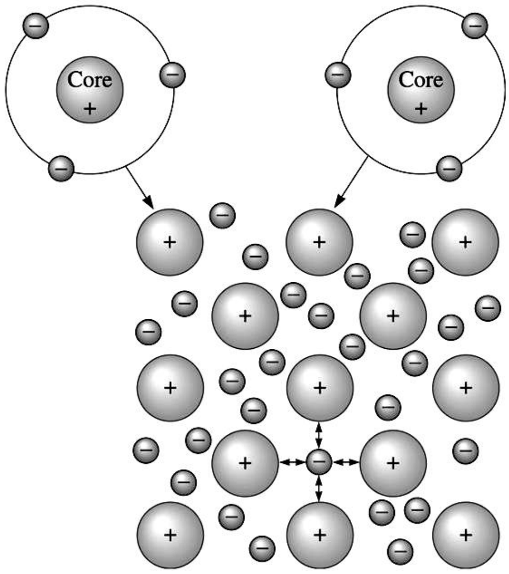
• Unsaturated C_nH_{2n}, C_nH_{2n-2}

- generally more reactive

Benzene (C_6H_6)
important for some polymeric materials



3. Metallic (large interatomic forces) nondirectional
metallic bond forms when atoms give up their valence electrons, 1, 2 or 3 from each atom, which then form an electron sea. The positively charged atom cores are bonded by mutual attraction to the negatively charged electrons. As the bond is not polar, metals are ductile.



• ***Secondary atomic and molecular bonds***
Fluctuating or permanent dipoles (also called **physical bonds,or van der Waals bonds or forces)**

- weak relatively to the primary bonding (2-5eV/atom or ion)

~ 0.1eV/atom or ~ 10 kJ/mol

- always present, but overwhelmed by other interaction most easily observed in inert gases
- dipoles to be considered

1. Permanent dipole bonds
2. Fluctuating dipole bonds

(Common, but weaker than primary bonding)

Dipole-dipole
H-bonds
Polar molecule-induced dipole
Fluctuating dipole (weakest)