

ESE 2019

UPSC ENGINEERING SERVICES EXAMINATION

Preliminary Examination

General Studies and Engineering Aptitude

Basics of Material Science and Engineering

Comprehensive Theory *with* Practice Questions
and ESE Solved Questions



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ESE 2019 Preliminary Examination : Basics of Material Science and Engineering

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Preface

The compilation of this book **Basics of Material Science and Engineering** was motivated by the desire to provide a concise book which can benefit students to understand the concepts of this specific topic of General Studies and Engineering Aptitude section.



B. Singh (Ex. IES)

This textbook provides all the requirements of the students, i.e. comprehensive coverage of theory, fundamental concepts and objective type questions articulated in a lucid language. The concise presentation will help the readers grasp the theory of this subject with clarity and apply them with ease to solve objective questions quickly. This book not only covers the syllabus of ESE in a holistic manner but is also useful for many other competitive examinations. All the topics are given the emphasis they deserve so that mere reading of the book clarifies all the concepts.

We have put in our sincere efforts to present detailed theory and MCQs without compromising the accuracy of answers. For the interest of the readers, some notes, do you know and interesting facts are given in the comprehensive manner. At the end of each chapter, sets of practice question are given with their keys and detailed explanations, that will allow the readers to evaluate their understanding of the topics and sharpen their question solving skills.

Our team has made their best efforts to remove all possible errors of any kind. Nonetheless, we would highly appreciate and acknowledge if you find and share with us any printing and conceptual errors.

It is impossible to thank all the individuals who helped us, but we would like to sincerely thank all the authors, editors and reviewers for putting in their efforts to publish this book.

With Best Wishes

B. Singh

CMD, MADE EASY Group

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2.1 Basic Laws of Chemistry

Atomic mass unit

It is defined as a mass exactly equal to one-twelfth the mass of one carbon - 12 atoms.

$$1 \text{ amu} = 1.66056 \times 10^{-24} \text{g}$$

Mole

The mole is unit of measurement for mass of substance in the International System of Units (SI).

"One mole is the amount of a substance that contains as many particles or entities as there are atoms in exactly 12 g (or 0.012 kg) of the ^{12}C isotope".

$$1 \text{ mole} = 6.023 \times 10^{23} \text{ atoms}$$

The mass of one mole of a substance in grams is called molar mass.

Avogadro number

In 1811, Avogadro proposed that equal volumes of gases at the same temperature and pressure should contain equal number of molecules. The number of entities or atoms in a mole is termed as Avogadro number, denoted by N_A .

$$N_A = 6.023 \times 10^{23} \text{ atoms/mol}$$

Law of conservation of mass

Antoine Lavoisier in 1789 stated that:

- "Matter can neither be created nor destroyed by chemical reactions or physical transformations."
- He performed careful experimental studies for combustion reactions for reaching to the above conclusion.
- According to this in a closed system for chemical reaction, the mass of the products must be equal to the mass of the reactants.

Law of Definite Proportions

A French chemist, Joseph Proust stated that:

- "A given compound always consist exactly the fixed and same proportion of elements by mass." It is sometimes also referred as Law of definite composition.
- An example is CO_2 . This gas is produced from a variety of reactions, often by the burning of materials, wood or fossil fuels. The structure of the gas always consists of one atom of carbon and two atoms of oxygen.

Law of Multiple Proportions

John Dalton proposed this law in 1803, he states that:

- When two elements combine to form more than one compound, the mass of one element that combines with a fixed mass of the other element, will always be in a ratio of whole numbers.

Example: Hydrogen combines with oxygen to form two compounds, named as water and hydrogen peroxide.

Hydrogen (2g) + Oxygen (16g) \rightarrow Water (18g)

Hydrogen (2g) + Oxygen (32g) \rightarrow Hydrogen Peroxide (34g)

Here, the masses of oxygen (16 g and 32 g) which combine with a fixed mass of hydrogen (2g) bear a simple ratio, i.e. 16:32 or 1:2.

2.2 Fundamental Concepts

- A substance which can not be decomposed into other substances is known as element. The smaller particle of an element which takes part in chemical reaction is known as an atom.
- An atom consists of a very small nucleus at its centre which is composed of protons and neutrons. The nucleus is encircled by moving electrons.
- The electron is a negatively charged particle and it has mass of about $1/1836$ that of the neutron. Proton has positive charge while a neutron is an uncharged particle having mass equal to the proton.
- Each chemical element is characterized by the number of protons in the nucleus or the **atomic number (Z)**. For an electrically neutral or complete atom, the atomic number also equals the number of electrons.
- The **atomic mass (A)** of a specific atom may be expressed as the sum of the masses of protons and neutrons within the nucleus.
- The atomic weight of an element corresponds to the weighted average of the atomic masses of the atom's naturally occurring isotopes. The **atomic mass unit (amu)** may be used for computations of atomic weight.

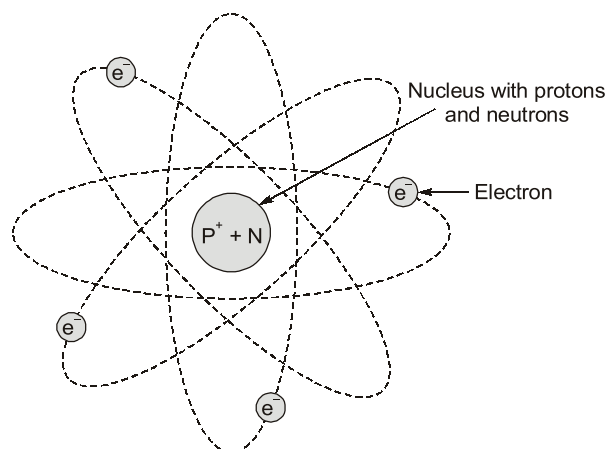


Fig. 2.1 Concept of an atom

NOTE



A scale has been established whereby 1 amu is defined as $1/12$ of the atomic mass of the most common isotope of carbon, (carbon -12, $A = 12.00000$). Within this scheme, the masses of protons and neutrons are slightly greater than unity and

$$A \cong Z + N$$

where N = Number of neutrons.

- **Isotopes:** Isotopes have different atomic weights but they have same atomic number. Isotopes are chemically inseparable as they possess identical chemical properties. Isotopes of the same element have the same atomic number and the same charge on the nucleus. ${}_1\text{H}^1$, ${}_1\text{H}^2$ and ${}_1\text{H}^3$ are isotopes of hydrogen while ${}_{17}\text{Cl}^{37}$ and ${}_{17}\text{Cl}^{35}$ are isotopes of chlorine.
- **Isobars:** Atoms which have same mass number (atomic weight or number of protons and neutrons) but they differ in atomic number are called isobars. Isobars are atoms of different chemical elements but they have same atomic mass number. Ar^{40} and Ca^{40} are isobars having same atomic mass number of 40 but they have varying number of protons (atomic number) and neutrons.

- **Isotones:** Atoms whose nuclei have the same number of neutrons but different number of protons. Thus, chlorine-37 and potassium-39 are isotones as their nuclei contain 17 and 19 protons respectively but same 20 neutrons. Isotones have different atomic number and different chemical properties.

2.3 Electrons in Atoms

- The electrons, protons and neutrons in atoms of various elements are identical. Thus, it follows that electrons, protons and neutrons are the fundamental particles of the universe. If it is so, then why do various elements behave differently? This is because of the difference in the number and arrangement of the electrons, protons and neutrons of which each atom is composed.
- All the electrons of an atom do not move in the same orbit. The electrons in an atom are arranged in different orbits or shells.



Remember

In general a shell (or orbit) can contain a maximum of $2n^2$ electrons, where n is the number of shell (or orbit). But according to this rule, there is an exception, the outermost orbit in an atom can not accommodate more than eight electrons. The electrons present in the outermost shell (or orbit) are called valence electrons.

- All the elements have been arranged in a periodic table according to the electronic arrangements in their atoms. The element placed in one vertical column have very similar properties.

2.4 The Periodic Table

- All the elements have been classified according to electron configuration in the **periodic table**. Here, the elements are situated, with increasing atomic number, in seven horizontal rows called periods.
- The arrangement is such that all elements arrayed in a given column or group have similar valence electron structures, as well as chemical and physical properties. These properties change gradually, moving horizontally across each period and vertically down each column.
- The elements positioned in Group 0, the rightmost group, are the inert gases, which have filled electron shells and stable electron configurations. Group VIIA and VIA elements are one and two electrons deficient, respectively, from having stable structures.
- The Group VIIA elements (F, Cl, Br, I and At) are sometimes termed the halogens. The alkali and the alkaline earth metals (Li, Na, K, Be, Mg, Ca etc.) are labeled as Groups IA and IIA, having, respectively, one and two electrons in excess of stable structures.
- The elements in the three long periods, Groups IIIB through IIB, are termed as the transition metals, which have partially filled d electron states and in some cases one or two electrons in the next higher energy shell.
- Groups IIIA, IVA and VA (B, Si, Ge, As etc.) display characteristics that are intermediate between the metals and nonmetals by virtue of their valence electron structures.
- As may be noted from the periodic table, most of the elements really come under the metal classification. These are sometimes termed **electropositive** elements, indicating that they are capable of giving up their few valence electrons to become positively charged ions.
- Furthermore, the elements situated on the right-hand side of the table are **electronegative**; that is, they readily accept electrons to form negatively charged ions or sometimes they share electrons with other atoms.
- Atoms are more likely to accept electrons if their outer shells are almost full and if they are less “shielded” from (i.e., closer to) the nucleus.

IA																		0						
1																		2						
H																		He						
1.0080																		4.0026						
IIA																		IIIA		IVA	VA	VIA	VIIA	
3	4																	5	6	7	8	9	10	
Li	Be																	B	C	N	O	F	Ne	
6.941	9.0122																	10.811	12.011	14.007	15.999	18.998	20.180	
11	12																	13	14	15	16	17	18	
Na	Mg																	Al	Si	P	S	Cl	Ar	
22.990	24.305	IIIB	IVB	VB	VIB	VIIB	VIII			IB	IIB	26.982	28.086	30.974	32.054	35.453	39.948							
19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36							
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr							
39.099	40.08	44.956	47.87	50.942	51.996	54.938	55.845	58.933	58.69	63.54	65.41	69.72	72.64	74.922	75.96	79.904	83.80							
37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54							
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe							
85.47	87.62	88.91	91.22	92.91	95.94	(98)	101.07	102.91	105.4	107.87	112.41	114.82	118.71	121.76	127.60	126.90	131.30							
55	56	Rare earth series		72	73	74	75	76	77	78	79	80	81	82	83	84	85	86						
Cs	Ba			Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn						
132.91	137.34			178.49	180.95	183.84	186.2	190.23	192.2	195.08	196.97	200.59	204.38	207.19	208.98	(209)	(210)	(222)						
87	88	Acti- nide series		104	105	106	107	108	109	110														
Fr	Ra			Rf	Db	Sg	Bh	Hd	Mt	Ds														
(223)	(225)			(261)	(262)	(266)	(264)	(227)	(268)	(281)														
Rare earth series		57	58	59	60	61	62	63	64	65	66	67	68	69	70	71								
		La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu								
		138.91	140.12	140.91	144.24	(145)	150.35	151.96	157.25	158.92	162.50	164.93	167.26	168.93	173.04	174.97								
Actinide series		89	90	91	92	93	94	95	96	97	98	99	100	101	102	103								
		Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr								
		(227)	232.04	231.04	238.03	(237)	(244)	(243)	(247)	(247)	(251)	(252)	(257)	(258)	(259)	(262)								

Fig. 2.2 The periodic table of the elements. The numbers in parentheses are the atomic weights of the most stable or common isotopes.

2.5 Comparison of Alpha (α), Beta (β) and Gamma (γ) Rays

2.5.1 Alpha Rays

- Alpha rays or alpha particles are the positively charged particles.
- These particles have highly active & energetic helium nucleus which contains two protons and two neutrons.
- Alpha particles have the least penetration power but the greatest ionization power.
- They cannot penetrate the skin but this does not mean that they are not dangerous. Since they have a great ionization power, so if they get into the body they can cause serious damage.

2.5.2 Beta Rays

- Beta particles are extremely energetic electrons that are liberated from the inner nucleus.
- They are negatively charged and have a negligible mass. On the emission of a beta particle, a neutron in the nucleus splits into a proton and an electron.
- Hence, it is the electron that is emitted by the nucleus at a rapid pace.
- Beta particles have a higher penetration power and lower ionization power when compared to alpha particles and can travel through the skin with ease.

2.5.3 Gamma Rays

- The waves arising from the high-frequency end of the electromagnetic spectrum that has no mass are known as gamma rays.
- They hold the highest power of penetration. They are the most penetrating but least ionizing and very difficult to resist them from entering the body.
- The Gamma rays carry a large amount of energy and can also travel via thick concrete and thin lead.

2.5.4 Properties of Alpha, Beta and Gamma rays

Table 2.1 Characteristics of Alpha, Beta and Gamma Rays

Characteristic	Alpha (α)	Beta (β)	Gamma (γ)
Emission of	$2P + 2N$	1 electron – High K.E.	Photon - very high frequency electromagnetic radiation
Changes from	Uranium to Plutonium	Radium to Polonium	No change
Charge (C)	+2	-1	0
Mass (amu)	4	1/1850	0
Speed km/s	15000	300000	300000
% of speed of light	5%	Close to 100%	100%
K.E.	3-6 MeV	5 MeV to 1 MeV	100 keV less than 10 MeV
Penetration Power	Low - Large mass & charge -can be stopped by a thin sheet of paper	Moderate - Medium mass and charge- can be stopped by a few mm thick metal	Very high - no mass, no charge, can be stopped only by a very thick cement or steel block
Ionization power	Very high - Large charge	Moderate - Low charge	Low - No charge

2.6 Quantum Number

Quantum numbers are used to find the electron configuration of an atom and the probable location, energy level, other characteristics like ionization and atomic radius of an electron in the atom. Quantum numbers are also applied to check the movement and orbit of each and every electron within an atom. Quantum numbers are of four types:

2.6.1 The principal quantum number (n)

- Principal quantum number of any electron in an atom stands for the main energy level or shell to which an electron belongs. Energy of an electron and its average distance from nucleus depends upon principal quantum number. Increasing the value of ' n ' results the distance of electron from its nucleus and its energy also start increasing.
- Shells are specified by a principal quantum number n , which may require an integral values beginning with unity; sometimes these shells are designated by the letters K, L, M, N, O and so on, which correspond, respectively to $n = 1, 2, 3, 4, 5, \dots$, shown in Table 2.2.

Table 2.2 Electron states in some of electron shells & subshells

Principal quantum Number (n)	Shell Designation	Subshells	No. of States	Number of Electrons	
				Per Subshell	Per Shell
1	K	s	1	2	2
2	L	s	1	2	8
		p	3	6	
3	M	s	1	2	18
		p	3	6	
		d	5	10	
4	N	s	1	2	32
		p	3	6	
		d	5	10	
		f	7	14	

2.6.2 The orbital angular momentum/ azimuthal quantum number (l):

l is the second quantum number which represents the sub-shell, denoted by letters s, p, d or f ; it is related to the shape of the sub-shell of electron. The number of these sub-shells is defined by the magnitude of n . It specifies the number of units of angular momentum connected with an electron in a given orbit and finds the shape of the orbit and the energy of the sublevel.

Note: For any value of n quantum number l can have any integral value from 0 to $n - 1$. Hence we can have $4d$, $5f$, $2p$ and $2s$ electrons whereas $1p$, $2d$, $3f$ subshells electrons do not exist.

Example: For

$$n = 1, \quad l = 0$$

$$n = 2, \quad l = 0, 1$$

$$n = 3, \quad l = 0, 1, 2$$

We have observed that n is the principal quantum number that defines principal shell. l provides the possible orbital sub-shells. The sub-shells in the main shell are s , p , d , f , g and h with quantum number $l = 0, 1, 2, 3, 4$ and 5 respectively. We can demonstrate it as follows:

For $n = 1, l = 0$, the electron is said to be in $1s$ sub-shell

$n = 2, l = 1$, the electron is said to be in $2p$ sub-shell

$n = 2, l = 0$, the electron is said to be in $2s$ sub-shell

2.6.3 The magnetic quantum number (m_l)

The third quantum number m_l is used to determine the number of orbitals for each subshell. For an 's' subshell, there is a single energy state, whereas for p , d and f subshells three, five and seven states exist, respectively (Table 2.2).

- The value of m_l varies between $+l$ to $-l$ with zero and as we know that m_l have $(2l + 1)$ values for a given l . For any specific value of l , an electron may have integral values of its inner quantum number m_l from $+l$ through 0 to $-l$. Thus for $l = 2$, m_l can take on the values $+2, +1, 0, -1$ and -2 . Thus we get

$$\text{For } l = 0, \quad m_l = 0$$

$$l = 1, \quad m_l = -1, 0, 1$$

$$l = 2, \quad m_l = -2, -1, 0, +1, +2$$

2.6.4 The Magnetic Spin Quantum Number (m_s)

- The electron can spin either in the clockwise or anticlockwise direction and values of spin can be $+\frac{1}{2}$ and $-\frac{1}{2}$, depending upon the direction of spin. m_s is used to represent the spin of an electron.
- We need to remember that the three quantum numbers n , l and m_l can have the same values for two electrons in an atom and that these two electrons will have their spins oriented in opposite directions.

Example 1.

Write the four quantum numbers for each of the electrons in the outermost shell of a boron atom?

Solution:

For boron, $Z = 5$, obviously, it has 5 electrons in it. Out of these 2 are in K shell and remaining 3 in the L -shell of the 3 electrons in the L shell 2 are $2s$ electrons and 1 is a p electron. Hence the quantum numbers of the electrons in the L -shell are as follows:

n	l	m_l	m_s
2	0	0	$+\frac{1}{2}$
2	0	0	$-\frac{1}{2}$
2	1	0	$\pm\frac{1}{2}$

Example 2.

When the quantum number $l = 4$, the quantum number m_l takes the following number of values.

- (a) 8 (b) 10
(c) 9 (d) 5

Ans: (c)

$$m_l = (2l + 1) = 2 \times 4 + 1 = 9$$

2.7 Electron Affinity

- This is the amount of energy released, when an electron is added by a neutral atom.
- The energy required to transfer an electron from one atom to another atom is the difference between the ionization energy I_1 and the electronic affinity E_{12} of the respective atoms, $I_1 - E_{12}$.
- Chlorine has the highest electron affinity.

NOTE

1. Electron affinity decreases with increase in atomic radius.
2. Sign given to electron affinity is negative because energy is released.
3. When force of attraction decreases electron affinity decreases.

2.8 Electronegativity

- Electronegativity is a chemical property that defines the tendency of an atom to attract a bonding pair of electrons towards itself. When an element strongly attracts electrons then it means that element has high electronegativity.
- Electronegativity is a measure of the ability of an atom in a chemical compound to attract shared electrons to it.
- The higher the associated electronegativity number, the more an element or compound attracts electrons towards it.
- The electronegativity of any given element varies depending on the element to which it is bound.
- Caesium is the least electronegative element in the periodic table ($= 0.79$), while fluorine is most electronegative ($= 3.98$). Electro-positivity is opposite of electronegativity that is a measure of an element's ability to donate electrons.

2.9 Pauli's Exclusion Principle:

He stated that, "No two electrons within the same atom can have the same numerical values for their set of four quantum numbers." This principle states that each electron state can hold no more than two electrons, which must have opposite spins. Thus, s , p , d and f sub-shells may each accommodate a total of 2, 6, 10 and 14 electrons respectively.

- Two electrons in an atom cannot be in the same quantum state i.e., their quantum numbers must be different.
- Of the four quantum numbers at least one must be different for the two electrons. For example n , l , m_l may be the same for the two electrons in an atom but the fourth quantum number m_s must be different for the two electrons. If m_s have $+\frac{1}{2}$ for one electron then it must have $-\frac{1}{2}$ for the other.
- Maximum number of electrons for a shell will be $= 2n^2$ where n is the principal quantum number.

2.10 Auf-bau Principle

It is used to predict which electron shells will be filled first in an atom. According to this

- Electron fill up the lowest available energy level first before beginning to fill the next shell or this states “Electrons are filled in the orbit of atoms in increasing energy order.” That means lower energy level orbits will be filled first then electrons enters into higher energy order or level.
- For an atom to be in ground state the orbital of higher energy can be filled only when all the lower energy orbital are completely filled up. Order of increasing energy in orbital:

$$1s < 2s < 2p < 3s < 3p < 4s < 3d < 4p < 5s < 4d < 5p < 6s < 4f < 5d < 6p < 7s \dots\dots$$

Note: Electrons follow $(n + l)$ rule to fill the orbital. The orbital having smaller $(n + l)$ value will be filled first.

Example 3.

Electron will be filled first in which of these two orbits: 5f or 6d?

Solution:

For $5f: (n + l) = 5 + 3 = 8$

For $6d: (n + l) = 6 + 2 = 8$

So in this case when $(n + l)$ have same values then the electron will be filled first in the orbit which has smaller principle quantum number so 5f will be filled first.

2.11 Hund's Rule

Hund's Rule tells us about how the electrons in an atom should be placed into degenerate orbits.

- It demonstrates that, electrons should be placed into separate orbits before going into the same orbital twice.
- For filling up oxygen atom electrons in three p orbital, we first distribute them one in each orbit of p then we double the first orbit.

Every orbital in a sublevel is singly occupied before any orbital is doubly occupied. All of the electrons in singly occupied orbits have the same spin to maximize total spin.

Example 4.

How many unpaired electrons are there in a chromium atom?

Solution:

Chromium (24) = $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^4$ (Normal case)

Actual configuration = $1s^2 2s^2 2p^6 3s^2 3p^6 4s^1 3d^5$ (for Better stability),

There are 6 unpaired electrons.

2.12 Heisenberg Uncertainty Principle

Heisenberg in 1927 remarked that

- The wave representation of the particle implies some uncertainty Δx of the position x of the particle and a corresponding uncertainty Δp in specifying its momentum p simultaneously.
- He proposed the following relationship between uncertainties Δx and Δp :

$$\Delta x. \Delta p \geq \left(\frac{h}{4\pi} \right)$$

Here Δx is uncertainty in position, Δp is uncertainty in momentum and Planck's constant

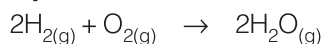
$$h = 6.6256 \times 10^{-34} \text{ J s.}$$

This is known as Heisenberg's uncertainty relation. This principle asserts that it is impossible to determine precisely both the position and momentum of a body in motion simultaneously.

2.13 Gay Lussac's Law of Gaseous Volumes

Gay Lussac in 1808 has observed that, when gases have chemical reactions, they do so in a simple ratio by volume. Provided all gases are at identical temperature and pressure.

Example:



2 vols. 1 vol. 2 vols.

2 volumes of hydrogen combine with 1 volume of oxygen to form 2 volumes of water.

2.14 Dalton's Atomic Theory

In 1808, Dalton published 'A New System of Chemical Philosophy' in which he stated that:

- Matter is made of very tiny particles called atoms.
- Atoms are indivisible structures.
- Atoms can neither be created nor destroyed.
- All atoms of a particular element are similar in all respects including identical mass, physical or their chemical properties.
- Atoms of different elements show different properties and they have different masses and different chemical properties.
- Compounds are formed when atoms of different elements combine in a fixed ratio.

2.15 Rutherford Model

Rutherford atomic model, also called solar or nuclear atom or planetary model of the atom, description of the structure of atoms proposed (1911) by the New Zealand-born physicist Ernest Rutherford.

On the basis of his famous alpha particle scattering experiment:

- The model described the atom as a dense, tiny, positively charged core called a nucleus, in which nearly all the mass is concentrated, around which the light negative elements, called electrons, propagate at some distance, similar to planets revolving around the Sun.
- Electrons being negatively charged and nucleus being a densely condensed mass of positively charged particles are held together by intense electrostatic force of attraction.
- This model failed in explaining atom stability and linear spectrum of atom.

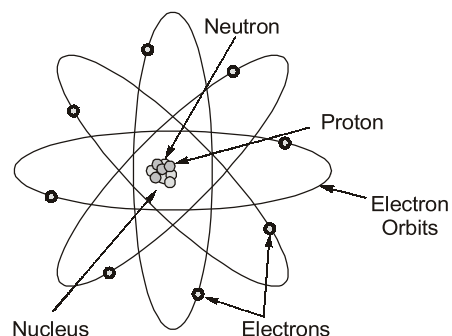


Fig.2.3 Rutherford Model

2.16 Bohr Model

Bohr Model is a modification of the earlier Rutherford Model; so it is also called as the Rutherford-Bohr Model.

- Bohr modified this atomic structure model by describing that electrons have motion in fixed shells for which the angular momentum of moving electron is an integral multiple of $\frac{h}{2\pi}$ and not anywhere in between and he also explained that each shell has a certain energy level.

- Bohr's model consists of a tiny nucleus (positively charged) surrounded by negative electrons revolving around the nucleus in orbits. Bohr found that electrons near to the nucleus have less energy and electron located away from the nucleus has more energy.
- The electrons in an atom shift from lower energy level to higher energy level by obtaining the required energy and an electron moves from higher energy level to lower energy level by losing energy. The amount of energy which an electron released or absorbed is the differences of the energies of the two orbits.

$$h\nu = E_2 - E_1$$

- Where h is Planck's constant, E_1 is the electron energy of lower orbit and E_2 is the electron energy of higher orbit.
- Bohr's model of an atom failed to explain Zeeman Effect (effect of magnetic field on the spectra of atoms).
- It also failed to explain the Stark effect (effect of electric field on the spectra of atoms).
- Bohr model could not explain the uncertainty principle of Heisenberg.
- Bohr Theory has no explanation for elliptical orbits.

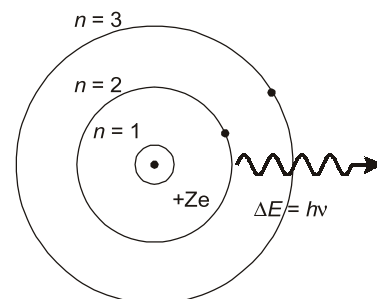


Fig. 2.4 Bohr Model

2.17 Sommer Field's Model

According to Sommer field,

- The path of an electron around the nucleus is an ellipse with the nucleus at one of its foci.
- The velocity of the electron revolving in an elliptical orbit varies at different parts of the orbit. This causes the proportional variation in the mass of the moving electron.

To deal with these two variables, two quantum numbers are introduced

- The principal quantum number n of Bohr's theory, which determines the energy of the electrons.
- A new quantum number called orbital or azimuthal quantum number (l) which has been introduced to characterise the angular momentum in an orbit i.e., it determines the orbital angular momentum of the electron. Its values vary from zero to $(n - 1)$ in steps of unity.

2.18 De Broglie Wave Equation:

In 1924 de Broglie suggested that

- Particles in motion should exhibit properties characteristic of waves. He further proposed that certain basic formulae should apply both to waves and particles.
- The wavelength of such particles e.g., electron, proton, neutron etc. is given by the relation

$$\lambda = \frac{h}{mv} \quad \dots (i)$$

Where h is Planck's constant, m is mass of the particle and v is the velocity of the particle. De Broglie called these waves as matter waves.

Relation (i) gives the mathematical relationship between the momentum ($p = mv$) of a particle which is a dynamical variable tendency of a corpuscle and the wavelength which is characteristic of the associated wave.

- The higher the energy of the electron, the greater will be its momentum mv and hence the smaller will be the wavelength of the wave function in terms of which its motion can be described.

2.19 Octet Rule

Gilbert N. Lewis formulated the "Octet rule" in 1916 which explains chemical combination between atoms known as electronic theory of chemical bonding. He stated that:

- Atoms will react to get in possibly the most stable state because a complete octet is very stable.
- Atoms can combine either by transfer of valence electrons from one atom to another (gaining or losing) or by sharing of valence electrons in order to have an octet in their valence shells.
- Atoms with greater stability have less energy, so a reaction that increases the stability of the atoms will release energy in the form of heat or light.

NOTE

The noble gases rarely form compounds. They have the most stable configuration (full octet, no charge), so they have no reason to change their configuration. All other elements attempt to gain, lose or share electrons to achieve a noble gas configuration.

2.20 Boyle's Law (Pressure - Volume Relationship)

Robert Boyle developed relationship of a gas with pressure and volume around 1660 and is known as Boyle's Law. According to this-

"At constant temperature, the pressure of a fixed amount of gas varies inversely with its volume."

Mathematically, it can be expressed as

$$P \propto \frac{1}{V} \quad (\text{at constant } T \text{ and } n)$$

$$P = \frac{k_1}{V}$$

k_1 is the constant which is also known as Boyle's constant and the value of k_1 depends upon the amount of the gas, temperature of the gas and the units in which P and V are expressed.

$$PV = k_1$$

It means that at constant temperature, product of pressure and volume of a fixed amount of gas is constant.

Suppose P_1 and V_1 are the initial pressure and volume of the given mass of gas. This gas now undergoes expansion at a fixed temperature and the pressure and volume changes to P_2 and V_2 . Now, According to Boyle's law:

$$P_1 V_1 = P_2 V_2 \quad (\text{at constant temperature})$$

2.21 Charles Law (Temperature - Volume Relationship)

Charles' law, which states that at constant pressure, the volume of a fixed mass of a gas is directly proportional to its absolute temperature. According to this:

- Volume of a gas increases on increasing temperature and decreases on cooling for a fixed mass of a gas at constant pressure.
- They found that for each degree rise in temperature, volume of a gas increases by $\frac{1}{273.15}$ of the original volume of the gas at 0 °C.

Let volumes of the gas at 0 °C and at t °C are V_0 and V_t respectively then,

$$V_t = V_0 + \left(\frac{t}{273.15} \right) V_0 \quad [\text{at constant } P]$$

⇒

$$V_t = V_0 \left(1 + \frac{t}{273.15} \right) = V_0 \left(\frac{273.15 + t}{273.15} \right)$$

At this stage, we define a new scale of temperature called the Kelvin temperature scale or Absolute temperature scale such that $t^{\circ}\text{C}$ on new scale is given by $T = (273.15 + t)\text{K}$ and 0°C will be given by $T_0 = 273.15\text{K}$. Thus 0°C on the Celsius scale is equal to 273.15K at the absolute scale. Kelvin scale of temperature is also called Thermodynamic scale of temperature.

Now Let us assume

$$T_t = (273.15 + t)\text{K and } T_0 = 273.15\text{K}$$

Then

$$V_t = V_0 \left(\frac{T_t}{T_0} \right)$$

Or,

$$\left(\frac{V_t}{V_0} \right) = \left(\frac{T_t}{T_0} \right)$$

We can write it as

$$\left(\frac{V_2}{V_1} \right) = \left(\frac{T_2}{T_1} \right)$$

$$\left(\frac{V_1}{T_1} \right) = \left(\frac{V_2}{T_2} \right)$$

\Rightarrow

$$\frac{V}{T} = \text{constant} = k_2$$

Hence,

$$V = k_2 T$$

The value of k_2 depends on the pressure of the gas, its amount and also on the unit of volume V .

OR

The volume of a gas varies directly with the temperature of the gas when the pressure of the gas is constant.

$$V \propto T \quad [\text{at constant } P]$$

\Rightarrow

$$\frac{V}{T} = \text{constant} = k_2$$

Note: The lowest hypothetical or imaginary temperature at which gases are supposed to occupy zero volume is called Absolute zero temperature.

2.22 Gay-Lussac's Law (Pressure - Temperature Relationship)

This law gives the relationship between the pressure and temperature of a fixed mass of gas at constant volume. This states that:

"For a fixed amount of gas, the pressure of the gas is directly proportional to its absolute temperature when its volume is kept constant." It can be expressed as

$$P \propto T \quad [\text{at constant } V]$$

\Rightarrow

$$\frac{P}{T} = \text{constant} = k_3$$

2.23 Avogadro Law (Volume - Amount Relationship)

In 1811 Italian scientist Amedeo Avogadro stated that:

The volume of a gas is directly proportional to the number of moles (or number of molecules) of gas when the temperature and pressure are held constant.

$$V \propto n \quad [\text{at constant } T \text{ and } P]$$

\Rightarrow

$$V = k_4 n$$

Where ' n ' is the number of moles of the gas and ' k_4 ' is a constant.

2.24 Ideal Gas Equation

The Ideal Gas Law is simply the combination of all Simple Gas Laws (Boyle's Law, Charles' Law and Avogadro's Law) that are

At constant T and n ; $V \propto \frac{1}{P}$ Boyle's Law

At constant P and n ; $V \propto T$ Charles' Law

At constant P and T ; $V \propto n$ Avogadro Law

So, $V \propto \frac{nT}{P}$

$\Rightarrow V = R \left(\frac{nT}{P} \right)$

R is proportionality constant or universal gas constant which has the same value for all gases.

Rearranging the above equation: $PV = nRT$

$\Rightarrow R = \frac{PV}{nT}$

2.25 Dalton's Law of Partial Pressures

John Dalton in 1801 states that "The total pressure exerted by the mixture of non-reactive gases is equal to the sum of the partial pressures of individual gases."

In a mixture of gases, the pressure exerted by the individual gas is called partial pressure. Mathematically,

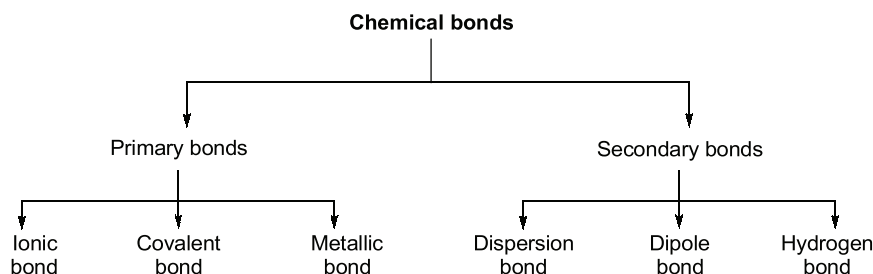
$$P_{\text{Total}} = P_1 + P_2 + P_3 + \dots \text{ at constant } T \text{ and } V$$

Where P_{Total} is the total pressure exerted by the mixture of gases and P_1, P_2, P_3 etc. are partial pressures of gases.

2.26 Chemical Bonding

- The atoms and molecules are held together by strong mutual forces of attraction. These interatomic forces are electrostatic in nature and depend upon the electronic structure of the element.

"Binding forces between atoms and molecules are known as chemical bonds."



- Primary bonds are interatomic bonds; these bonds are stable and strong.
- Secondary or molecular bonds are formed due to intermolecular attraction forces or vander Waals forces between molecules.
- The atoms or molecules which have their outermost shells completely filled have no tendency to gain, lose or share valence electrons. They have to depend upon Van der Waal's forces of attraction for bonding.
- Van der Waal's forces are due to the electrostatic attraction between nucleus of one atom and the electrons of the other atoms. These bonds are weak and unstable.

2.27 Ionic Bond

- An ionic bond is formed due to the attractive force between a positive ion and a negative ion when they are brought into close proximity.
- The ions are formed when the atoms involved either lose or gain electrons to stabilize their outer shell electronic configuration by forming ions. Electropositive elements tend to lose electrons while electronegative elements tend to gain electrons.
- The sodium (metal) has a single electron in the outer shell and it tends to lose it, thereby forming a positive ion (Na^+). The chlorine (non-metal) has seven electrons in the outer shell and it tends to gain a single electron for gaining stable configuration, thereby forming a negative ion (Cl^-).
- The positive ions and negative ions attract each other and bonds are formed by the electrostatic binding force as shown in figure 2.5. The chemical reaction can be given as:

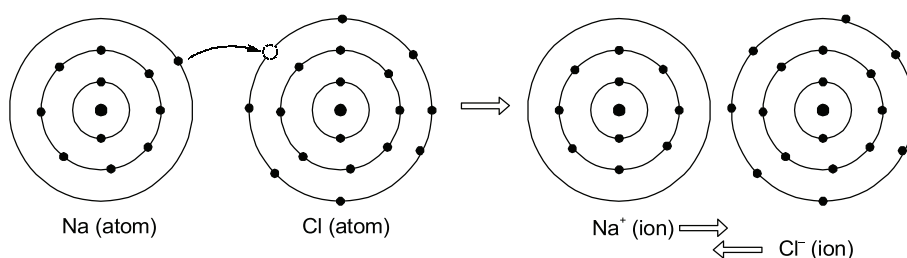
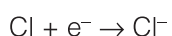


Fig. 2.5 Ionic bond by electrostatic binding force

- Ionic bonds are non-directional and they form compounds which have general characteristics as given below:
 - (i) Crystalline in nature
 - (ii) High strength
 - (iii) High hardness
 - (iv) Having high melting and boiling temperature due to strong electrostatic forces binding atoms.
 - (v) Have brittleness
 - (vi) Non-conducting of electricity

Ionic Radius:

- The removal of an electron from an atom results in the formation of a cation while gain of an electron leads to the formation of an anion.
- The ionic radii can be estimated by measuring the distances between cations and anions in ionic crystals.
- The size of an anion will be larger than the parent atom due to the addition of one or more electron will result in increased repulsion among the electrons and a decrease in effective nuclear charge.
- A cation is smaller than its parent atom because it has lesser electrons while its nuclear charge remains the same.

Example 1.

Explain why cations are smaller and anions are larger in radii than their parent atoms?

Solution:

Cations are smaller in size because they are formed by loss of electrons and anions are larger in size because they are formed by the gain of electrons.

OR

- Anions are always larger than their parent atoms because the addition of one or more electrons would result in increased repulsion among the electrons and a decrease in the effective nuclear charge. This is opposite in case of cations.
- Cations are always smaller than their parent atoms because they have lesser electrons, whereas their nuclear charge remains the same. The remaining electrons are, therefore held more tightly by the protons in the nucleus and thus their radii are smaller than the parent atoms.

2.28 Covalent Bond

- A covalent bond is formed by sharing of electrons between the atoms. The covalent bonds are formed between many non-metallic elements as the atoms of these elements, usually have incompletely filled outer electron orbits. Such elements are hydrogen, carbon, chlorine, nitrogen and oxygen.
- The formation of chlorine molecule by covalent bond is shown in figure 2.6. The outer shell of chlorine atom has seven electrons. When two chlorine atoms are brought closer, then each chlorine atom tries to gain one electron to form stable electronic configuration. This is achieved by a pair of chlorine atoms by sharing two electrons, thereby producing a stable diatomic molecule.
- Covalent bonds are directional in nature and covalent compound can be solids, liquids and gaseous. The compounds having covalent bond have following general characteristics:
 - (i) Like the ionic bond, the covalent bond tends to produce materials with high strength.
 - (ii) Have high melting and boiling temperature.
 - (iii) Atom movement within the material (deformation) requires the breaking of distinct bonds, thereby making the material characteristically brittle.
 - (iv) Electrical conductivity depends upon the bond strength, ranging from conductive tin (weak covalent bond) through semiconductive silicon and germanium to insulating diamond.
 - (v) Covalent solids do not form closed pack structures as bonding has directional nature.

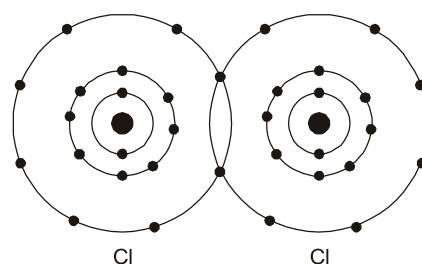


Fig. 2.6 Formation of a covalent bond (chlorine molecule)

Types of Covalent bond:

σ -(Sigma) bond

- It follows axial overlapping of orbitals. Bond formed by linear overlapping of half filled atomic orbital is called as sigma bond. A covalent bond results from the formation of a molecular orbital by the end-to-end overlap of atomic orbitals, denoted by the symbol σ . i.e. s , p along the same axis.

π bond

- Lateral overlapping of orbitals. It can be formed by overlapping of two adjacent half filled orbitals. When two orbital overlapping form π bond then at the time of overlapping these two orbitals form parallel axis to each other. A covalent bond resulting from the formation of a molecular orbital by side-to-side overlap of atomic orbitals along a plane perpendicular to a line connecting the nuclei of the atoms, denoted by the symbol π , i.e. only p orbital forms it at the angle called bond angle.

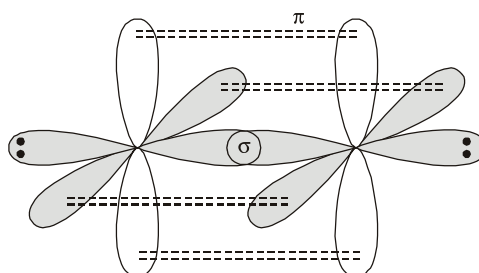


Fig. 2.7 Orbital structure of CO

- Hybrid bonds are formed when interaction between s and p sub orbitals occur. Double & triple bonds are unsaturated while single bonds are saturated.

Covalent Radius

- Covalent bond radius refers to half of the distance between two singly bonded atoms of the same element or we can define it as half the covalent bond length when the two atoms bonded are homonuclear. r_{cov} is typically measured by X-ray diffraction.

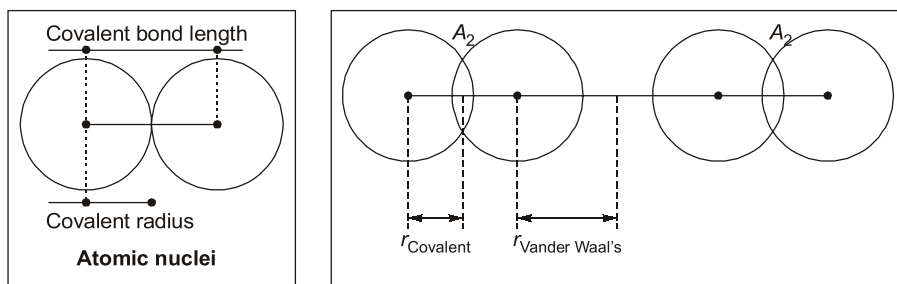


Fig.2.8 Covalent Radius

2.29 Metallic Bond

- A metallic bond is formed by the partial sharing of valence electrons by the neighbouring atoms. The atoms in metals and alloys are held together by such bonds. The elements having small number of loosely held valence electrons can easily release these electrons to the common pool.
- The bonding takes place when each atom contributes its valence electrons to the formation of an electron cloud and change into positive ions. The valence electrons are no longer bonded directly to any individual atom but they move freely in the sphere of influence of other atoms.
- It means that valence electrons are bonded to different atoms at different times and this binding lasts for a short time.
- Metallic bonding constitutes the electrostatic attraction forces between the delocalized electrons (electron cloud) and the positively charged metal ions.
- Bonding can be understood as the sharing of free electrons among a lattice of positively charged ions (cations). In metallic bonding, electrons are released from atoms, thereby leaving metal cations surrounded by a "sea of delocalized electrons" as shown in figure 2.9.

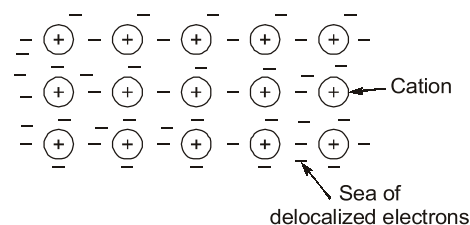


Fig.2.9 Metallic bonding

- The metallic bonding in metals and alloys provides the properties as per Table 2.3.

Table 2.3 Related metal properties due to metallic bonding

Property		Explanation
1.	Electrical conductivity	Electrons are free to move through cations lattice, thereby providing electricity carrier.
2.	Lustre	Light is reflected by the sea of delocalized electrons, thereby metal shines, i.e., it has lustre.
3.	Malleability and ductility	Metallic bonding is non-directional. Lattice of cations can be deformed and mobile electrons continue to hold the metal structure together.
4.	High melting and boiling points	Attraction between cation and electron cloud is strong.
5.	High density	Cations are closely packed in a three-dimensional network.

2.30 Comparison of Primary Bonds

- The comparison of primary bonds is as per Table 2.4.

Table 2.4 Comparison of primary bonds

S.No.	Characteristics	Ionic bond	Covalent bond	Metallic bond
1.	Bond energy	Higher than metallic	Higher than metallic	Generally lower than other primary bonds
2.	Nature of bond	Non-directional	Directional	Non-directional
3.	Examples	NaCl, MgO and CaF_2	Diamond, silicon germanium etc.	Molecules of Al, Cu, Mg and Ag
4.	Bond formation	Transfer of electrons	Sharing of electrons	Formation of electron cloud and cations
5.	Bonding force	Electrostatic force between anions and cations	Electrostatic force of attraction between two atoms	Electrostatic force between electron cloud and cations
6.	Conductivity	Low	Moderate	High
7.	Melting and boiling temperature	High	High	High
8.	Mechanical properties	High hardness	Hard	Good strength and ductility

2.31 Van der Waal Bond

- Van der Waals bond exists between two closed configuration atoms or between molecules and it is relatively a weak bond. The bond is due to dipole-dipole interaction.
- Van der Waals forces are a result of electrostatic attraction between temporary dipoles and induced dipoles caused by motion of electrons in atoms and molecules.
- Van der Waals forces are forces that occur between molecules of the similar substance. They are quite different from the forces that make up the molecule.
- The strength of Van der Waals forces is related to the size of atoms and molecules. Bigger the atom or molecule responds to the bigger Van der waals force.

Atomic Radius:

- It is generally stated as the total distance from an atom's nucleus to the outermost orbital of electron.
- In simpler terms, it can be defined as something similar to the radius of a circle, where the centre of the circle is the nucleus and the outer edge of the circle is the outermost orbital of electron.
- Atomic radius is measured in picometers (pm) or angstroms (\AA).

- An atom gets larger or the radius of atoms increases as the number of electronic shells increase; therefore the radius of atoms increases as you go down in a certain group in the periodic table of elements.
- In general, the size of an atom will decrease as you move from left to the right of a certain period.

Van der Waal Radius:

It is defined as half of the inter nuclear separation of two non-bonded atoms of the same element on their closest possible approach and is denoted r_v .

Note: It is important that two atoms does not share a chemical bond (e.g., O_2 , H_2) because the bond implies an overlap of the electron shells or a shared outer shell.

2.32 Dispersion Bonds

- In a symmetrical molecule, the electrons are distributed uniformly around the nucleus and the electrons are constantly rotating about nucleus. In a symmetrical molecule, the centres of positive charges and negative charges coincide with each other.
- However, in molecules where the distribution of electrons is not symmetrical about their nuclei. This causes the displacement between the centres of positive and negative charges as shown in figure 2.10.
- It creates electronic imbalance of the charge and this is called polarization. This polarization fluctuates with motion of electrons and is known as dispersion effect.
- Dispersion effect produces a weak force of attraction between two molecules of the same element and this bonding is called dispersion bond. Such bond is found in noble gases like argon, helium and neon etc.

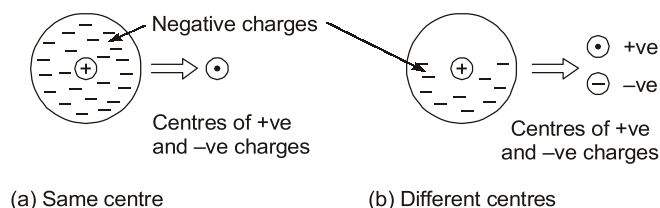
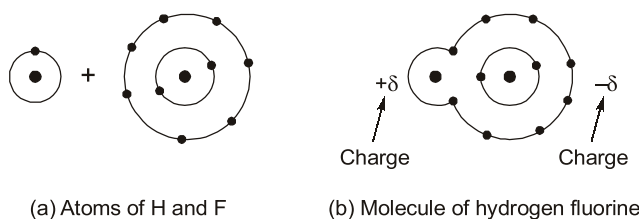
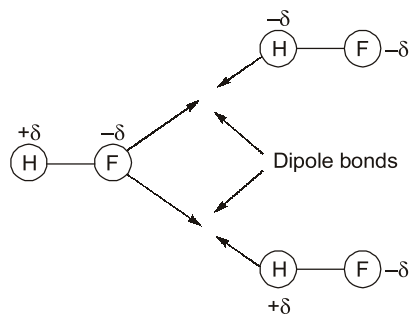


Fig. 2.10 Dispersion effects

2.33 Dipole Bonds

- In covalent bonding, there may be unequal sharing of electrons between two atoms forming molecules. This happens if one of the atoms has high affinity to attract electrons than the other atoms.
- The unequal sharing of electrons creates opposite charges on the molecules. As a result, permanent dipoles are produced. These dipoles attract each other, thereby forming dipole bonds.
- Dipole bonds are weaker than primary bonds but they are stronger than dispersion bonds.
- Hydrogen fluoride molecule has dipole bond as shown in figure 2.11.
- Fluorine atom has higher affinity than the hydrogen atom. Due to this, the shared electron pair shifts towards the fluorine atom in the covalent bonding. The shifting of electron pair produces a dipole with positive charge towards hydrogen atom and negative charge towards fluorine atom. The resulting dipoles produce necessary attraction to produce dipole bonding of molecules.



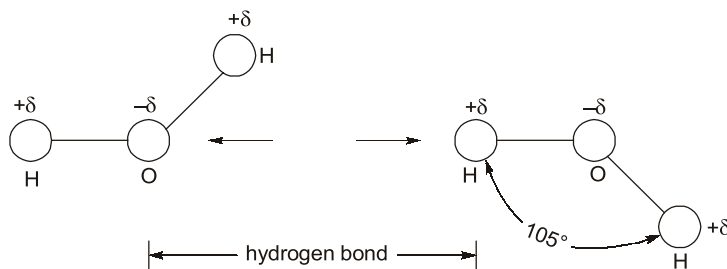


(c) Molecules forming dipole bonds

Fig. 2.11 Formation of dipole bonds

2.34 Hydrogen Bonds

- Hydrogen bond is a special type of dipole bond and it is produced between covalently bonded hydrogen atoms and oxygen, fluorine or nitrogen atoms.
- These atoms [F, O, N] have higher affinity for the shared electron pairs than hydrogen atoms. The shared electron pair shifts towards these higher electronegative atom. The shifting of electron pair produces a dipole. Similar dipoles are produced in other molecules. These dipoles attract each other, thereby forming hydrogen bonding to produce water as shown in figure 2.12.

**Fig. 2.12** Hydrogen bond between the water molecules

Types of Hydrogen Bond

- Hydrogen bonds are electromagnetic attractions between the positive and negative poles of atoms that exist when a hydrogen (H) atom, covalently bound to a highly electronegative atom such as nitrogen (N), oxygen (O) or fluorine (F) experiences electrostatic field of another nearby highly electronegative atom.

There are two types of H-bonds:

- Intermolecular Hydrogen Bond:** It is formed between two different molecules of the same or different compounds. These compounds have higher melting and boiling point.

Example: H-bond in case of HF molecule, NH_3 , alcohol or water molecule.

- Intramolecular Hydrogen Bond:** It is formed when hydrogen atom is in between the two highly electronegative (F, O and N) atoms present within the same molecule.

Ex.: In ortho nitro-phenol the hydrogen is in between the two oxygen atoms ortho chlorophenol etc.

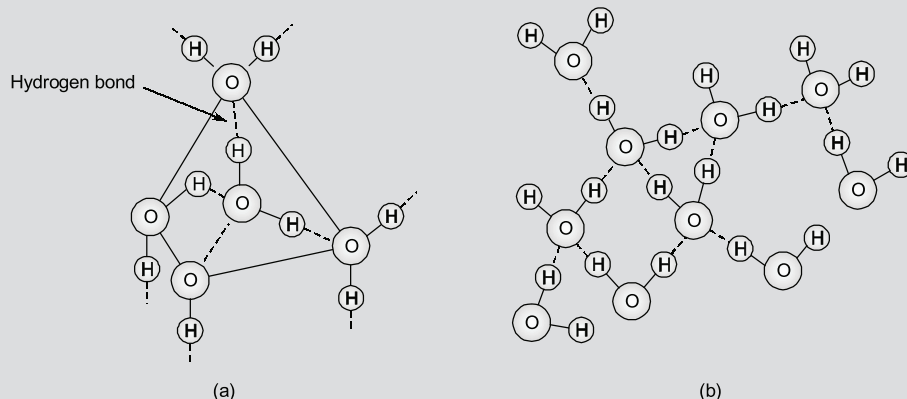
2.35 Properties of Water (H_2O)

- Water molecules are the only substance that exists in all three physical states of matter: solid, liquid and gas.
- Water has a high specific heat which is the amount of energy needed to change the temperature of a unit substance by 1°C .

- Water in a pure state has a neutral pH. So pure water is neither acidic nor basic. Rain has a naturally acidic pH of about 5.6 because it contains natural derived carbon dioxide and sulphur dioxide.
- Due to the difference in electro negativity, there is a bond dipole moment pointing from each H to the O , making the oxygen partially negative and hydrogen partially positive so the polar nature water has high adhesion properties.
- Water conducts heat more easily than any liquid except mercury.
- Water molecules exist in liquid form over the range of temperature from $0 - 100^{\circ}\text{C}$. 0° on the Celsius scale is water's freezing point and 100°C is water's boiling point.
- Water is a universal solvent. It is able to dissolve a large number of different chemical compounds.
- Water has a high surface tension. In other words, water is adhesive and elastic and tends to aggregate in drops rather than spread out over a surface as a thin film. Surface tension is responsible for capillary action, which allows water to move through the roots of plants and through the tiny blood vessels in our bodies.
- The freezing of water molecules causes their mass to occupy a larger volume. Fresh water has a maximum density at around 4°C .
- Water molecules does not deviate in magnetic field but due to the presence of electric dipoles they are deviated in electric field.

**Do
You
Know**

Upon freezing (i.e., transforming from a liquid to a solid upon cooling), most substances experience an increase in density (or, correspondingly, a decrease in volume). One exception is water, which exhibits the anomalous and familiar expansion upon freezing. This behavior may be explained on the basis of hydrogen bonding. Each molecule has two hydrogen atoms that can bond to oxygen atoms; in addition, its single O atom can bond to two hydrogen atoms of other molecules. Thus, for solid ice, each water molecule participates in four hydrogen bonds as shown in the three-dimensional schematic of figure (a); here hydrogen bonds are denoted by dashed lines and each water molecule has 4 nearest-neighbor molecules. This is a relatively open structure; i.e., the molecules are not closely packed together; and, as a result, the density is comparatively low. Upon melting, this structure is partially destroyed, such that the water molecules become more closely packed together as in figure (b); at room temperature the average number of nearest-neighbour of water molecules has increased to approximately 4.5; this leads to an increase in density.



The arrangement of water (H_2O) molecules in (a) solid ice and (b) liquid water

2.36 Directional Bond

- The meaning of bonds being directional is that atoms bonded covalently prefer specific orientations in space relative to one another.
- The bond forms at some angle called bond angle. As a result, molecules in which atoms are bonded covalently have specific shapes.
- The cause for this directionality is that bonds are made by sharing electrons between atoms or in other words, by overlapping the atomic orbitals of participant atom and usually only few patterns of overlap are possible, accordingly, only few spatial arrangements of atom are possible.
i.e. Hydrogen bond, covalent bond

2.37 Non-directional Bond

- There is no preferred direction for the bonds.
- Non-directional bonding is the bonding which includes opposite charges such as metallic and ionic.
- For instance, a metal cation in a metallic lattice will attract electrons from all directions with a uniform force and these electrons can rotate and the force of attraction will remain the same, so we say that there are non-directional forces of attraction between them, because the force does not favour any specific direction. i.e. ionic, metallic and Van der Waal's bond etc.

2.38 Molecular Orbital Theory

- While an electron in an atomic model is regulated by one nucleus, in a molecular orbit. It is influenced by two or more nuclei depending upon the number of atoms in the molecule. The number of molecular orbital formed is equal to the number of combining atomic orbitals.
- When two atomic orbitals combined together then two molecular orbital is formed. One is known as bonding molecular orbital and the other is known as anti bonding molecular orbital.
- Bonding molecular orbital have lower energy and hence greater stability than anti bonding molecular orbital.
 - Molecular orbital (MO) theory is a method for determining molecular structure in which electrons are not assigned to individual bonds between atoms, but are treated as moving under the effect of the nuclei in the whole molecule.
 - Molecular orbital (MO) theory uses a linear combination of atomic orbitals to represent molecular orbitals resulting from bonds between atoms. These are often divided into bonding orbitals, anti-bonding orbitals and non-bonding orbitals.
- A **bonding orbital** concentrates electron density in the region between a given pair of atoms, so that its electron density will tend to attract each of the two nuclei toward each other and hold the two atoms together.
- An **anti-bonding orbital** concentrates electron density behind each nucleus (i.e. on the side of each atom which is farthest from the other atom) and so tends to pull each of the two nuclei away from the other and actually weaken the bond between the two nuclei. They have higher energy than atomic orbitals.
- **Stability of molecules:** If N_b is the number of electrons occupying bonding orbitals and N_a is the number of electrons occupying anti bonding orbitals then, the molecule is stable if $N_b > N_a$; more bonding order are occupied and so the bonding influence is stronger and a stable molecule results.
- The molecule is unstable if $N_b \leq N_a$; the anti bonding influence is stronger and therefore the molecule is unstable.

- **Bond order:** It is defined as half of the difference between the number of electrons present in bonding and anti bonding orbitals.

$$\text{Bond order} = \frac{1}{2}(N_b - N_a)$$

2.39 Hybridization

- Hybridization occurs when an atom bonds using electrons from both the s and p orbitals, creating an imbalance in the energy levels of the electrons. To equalize these energy levels, the s and p orbitals involved are combined to create hybrid orbitals.

OR

- Hybridization is the process of mixing of standard atomic orbitals to form new orbitals of equal energy- which can be used to describe bonding in molecules.

Properties:

- In hybridization process atoms have approximately equal level of energy orbitals.
- Hybrid orbitals are similar in energy level and shape.
- Number of new hybrid orbitals will be equivalent to number of orbitals participating in the process of hybridization.
- Hybrid orbitals make sigma bond.
- Different hybrid orbitals have different geometrical shape and structure that depends upon type of hybridization.
- To find out the bond angle between two hybrid orbitals, we have

$$m = -\frac{1}{\cos \alpha}$$

α = Angle between two hybrid orbitals

m = Number of 'p' orbitals taking part in hybridization

i.e. sp^3 hybridization: $\cos \alpha = -\frac{1}{3} = 109^\circ 28'$

sp^2 hybridization: $\cos \alpha = -\frac{1}{2} = 120^\circ$

sp hybridization: $\cos \alpha = -\frac{1}{1} = -1 = 180^\circ$

Types of Hybridization:

1. **sp hybridization:** When one 's' orbital and one 'p' orbital mixed together to form 2 sp hybrid orbital that have bond angle of 180° then it is known as sp hybridization.
It is also called as linear hybridization due to having the linear shape of atoms.
Example: $BeCl_2$, BeF_2 , CO_2
2. **sp^2 hybridization:** When one 's' orbital and two 'p' orbitals mixed together to form 3 sp^2 hybrid orbitals that consist bond angle of 120° then it is known as sp^2 hybridization. sp^2 hybrid atoms have geometrical shape as trigonal planar.
Example: BF_3 , $SnCl_2$, C_2H_4
3. **sp^3 hybridization:** When one s orbital and three p orbitals mixed together to form 4 sp^3 hybrid orbitals that consist of bond angle of $109^\circ 28'$ then it's known as sp^3 hybridization. sp^3 hybrid atoms have geometrical shape as tetrahedral.
Example: NH_3 , $SiCl_4$, $CHCl_3$, CH_4