CSIR NET UNIT 1(A) Notes – Structure of Atoms, Molecules & Chemical Bonds – Download FREE PDF

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Atom is a basic unit of matter that consists of a dense central nucleus surrounded by a cloud of negatively charged electrons**.** Atoms are composed of three particles i.e. protons, electrons, and neutrons. Protons and neutrons are present inside the nucleus which account for the mass of the atom. Whereas electrons are present in the space around the nucleus (**Fig-1**). The number of electrons in the atom is equal to the number of protons. Atoms are extremely small.

Protons (p+) carry a positive charge with mass value of 1.672623 x 10-24 g and relative mass value of 1.007 atomic mass units (amu) but we can round to 1. **Electrons (e–)** carry a negative charge with mass value of 9.110 x 10-28 g and relative mass value of 0.0005 amu but we can round to 0. **Neutrons (no)** carry neutral charge with mass value of 1.6750 x10 -24 g and relative mass value of 1.009 amu but we can round to 1 (**Fig-2**). CSIR NET UNIT 1 Notes by Biotecnika – FREE PDF Download.

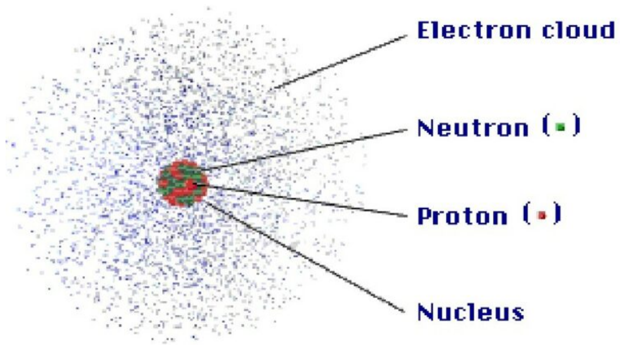


Fig-1: Atomic structure (Erwin Schrodinger electron cloud model)

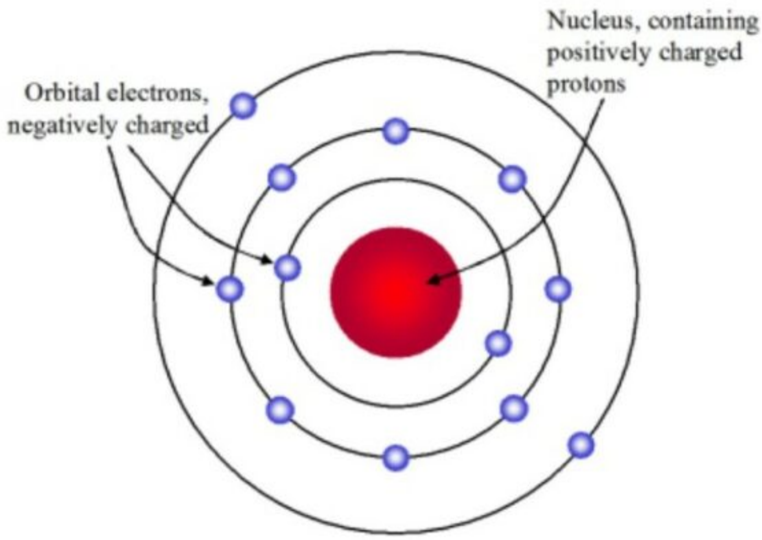


Fig-2: Atom with a positively charged nucleus and surrounding negatively charged orbital electrons

Atoms are consisting of protons and neutrons. Proton is a positive charge and neutron is a neutral charge i.e zero charges there is no charge in it.

ATOMIC STRUCTURE

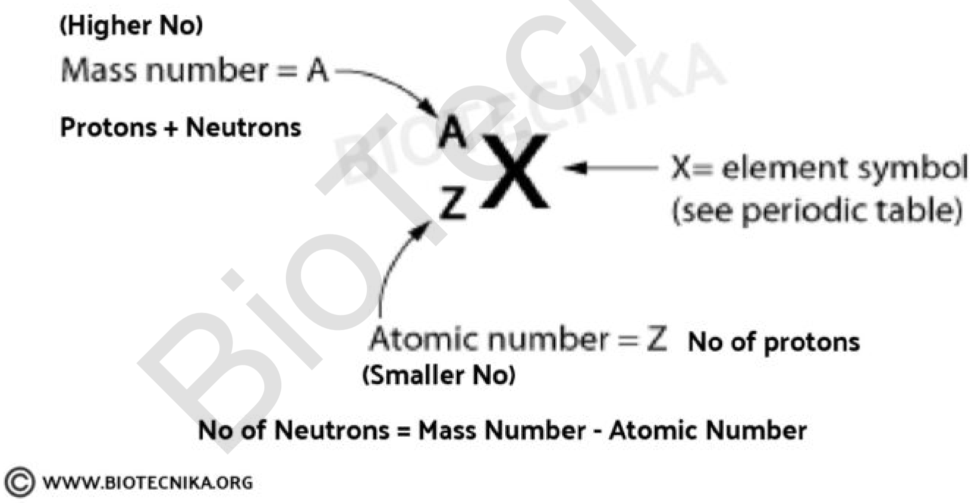
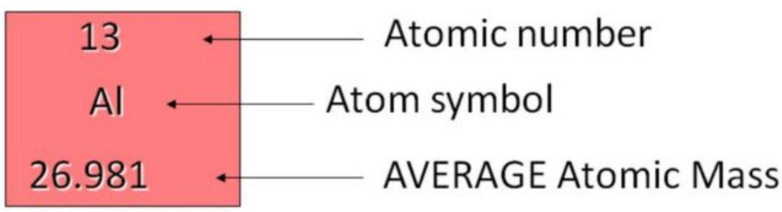


Fig 3: Atom Structure Representation & How To Calculate the Neutron No.



Atomic No, Z – All atoms of the same element have the same number of protons in the nucleus

Mass Number, A

- C atom with 6 protons and 6 neutrons is the mass standard

- = 12 atomic mass units
- Mass Number (A)= # protons + # neutrons
- NOT on the periodic table…(it is the AVERAGE atomic mass on the table)
- A boron atom can have A = 5 p + 5 n = 10 amu

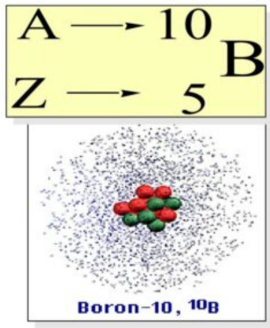


Fig 4: Boron

Isotopes

Isotopes are where you have different forms of an element having different neutron numbers because proton numbers cannot change. photon number if it changes the element only will change.

Now, like this many elements will be having isotopes, sometimes isotopes might be a little bit unstable in the nucleus for example, if you're taking tritium now, how many protons are there in tritium? It's one only since it's hydrogen isotope and how many neutrons are there two neutrons are there. If you do three minus one you will get two right. So, three minus 122 neutrons are there and one proton is there which means the neutron is more than the proton. So, this way the nucleus is a bit unstable. CSIR NET UNIT 1 Notes by Biotecnika – FREE PDF Download. So, it wants to give away some of its energy means, it wants to make itself stable by giving away some amount of energy and that is what is called radioactivity.

Atoms of the same element (same Z) but a different mass number (A).
• Boron-10 (10B) has 5 p and 5 n
• Boron-11 (11B) has 5 p and 6 n

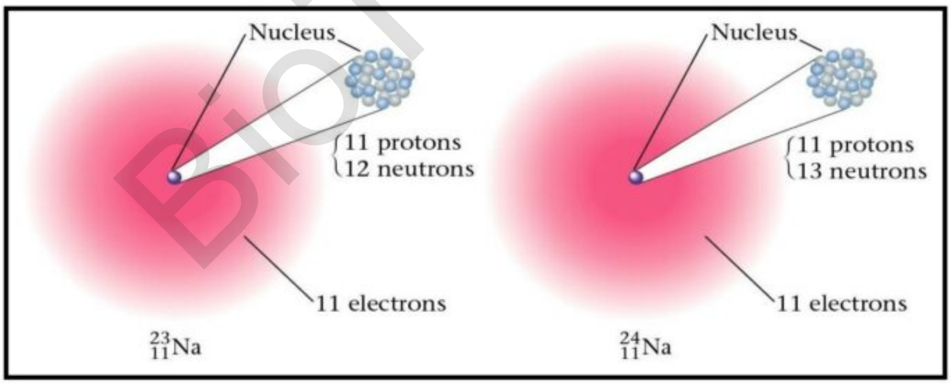


Fig 5: Two isotopes of Sodium

AVERAGE ATOMIC MASS

Average of all the isotopes that you have you have many isotopes of an element right. So, including all the isotopes whatever will be the total mass number is called the average atomic mass.

For eg: Boron, You will find two types of boron one is 10 boron – the one where you have five protons and five neutrons, and the other boron you see is 11 boron where five protons are fixed but you have six neutrons.

- Because of the existence of isotopes, the mass of a collection of atoms has an average value.
- Boron is 20% 10B and 80% 11B. That is, 11B is 80 percent abundant on earth
- For boron atomic weight = 0.20 (10 amu) + 0.80 (11 amu) = 10.8 amu

Isotopes & Their Uses

- Radioactive isotopes have an unstable nucleus that decays or emits excess energy or radiation until the nucleus becomes stable. They can be naturally occurring or artificial isotopes of an element. Bone scans with radioactive technetium-99.
- The tritium content of groundwater is used to discover the source of the water, for example, in municipal water or the source of the steam from a volcano.

Radioactive Isotope	Applications in Medicine
Cobalt-60	Radiation therapy to prevent cancer
Iodine-131	Locate brain tumors, monitor cardiac, liver and thyroid activity
Carbon-14	Study metabolism changes for patients with diabetes, gout and anemia
Carbon-11	Tagged onto glucose to monitor organs during a PET scan
Sodium-24	Study blood circulation
Thallium-201	Determine damage in heart tissue, detection of tumors
Technetium-99m	Locate brain tumors and damaged heart cells, radiotracer in medical diagnostics (imaging of organs and blood flow studies)

Radioactive Isotope	Application in Research
Carbon-14	Carbon dating of organisms and substances (archeology), research to determine steps involved in plant photosynthesis
Phosphorus-32 Phosphorus-33	Used in research involving biology and genetics
Selenium-75	Protein studies in life science
Strontium-85	Metabolism and bone formation studies
Hydrogen-3 or Tritium	Used to study life science and drug metabolism

Fig 6: Radioisotopes & their use

Practice Question: From CSIR NET Question Paper of Dec 2016

From the following statements,
A. Hydrogen, Deuterium, and Tritium differ in the number of protons
B. Hydrogen, Deuterium, and Tritium differ in the number of neutrons
C. Both Deuterium and Tritium are radioactive and decay into Hydrogen and Deuterium, respectively
D. Tritium is radioactive and decays to Helium
E. Carbon-14 decays to Nitrogen-14
F. Carbon-14 decays to Carbon-13

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Pick the combination with ALL correct statements.
1. A, B, and F
2. B, D, and E – **Correct Answer**
3. A, C, and D
4. C, E, and F

IONS

Ions are atoms or groups of atoms with a positive or negative charge. Taking away an electron from an atom gives a **Cation** with a positive charge. Adding an electron to an atom gives an **Anion** a negative charge. In order to show the difference between an atom and an ion, the charge is mentioned in the superscript of an ion.

Examples: Na+ Ca+2 I– O-2

Forming Cations & Anions

- A CATION forms when an atom loses one or more electrons.
- An ANION forms when an atom gains one or more electrons

Electronegativity

The ability of an atom in a molecule to attract electrons to itself.

Electronegativity is a function of two properties of isolated atoms:

- The atom's ionization energy (how strongly an atom holds onto its own electrons)
- The atom's electron affinity (how strongly the atom attracts other electrons)

Prof. Linus Pauling
Nobel Prize for Chemistry 1954
Nobel Prize for Peace 1962

Fig 7: Prof Linus Pauling

For example, an element that has:

- A large (negative) electron affinity
- A high ionization (always endothermic, or positive for neutral atoms)
- Will: Attract electrons from other atoms and Resist having electrons attracted away
- Such atoms will be highly electronegative
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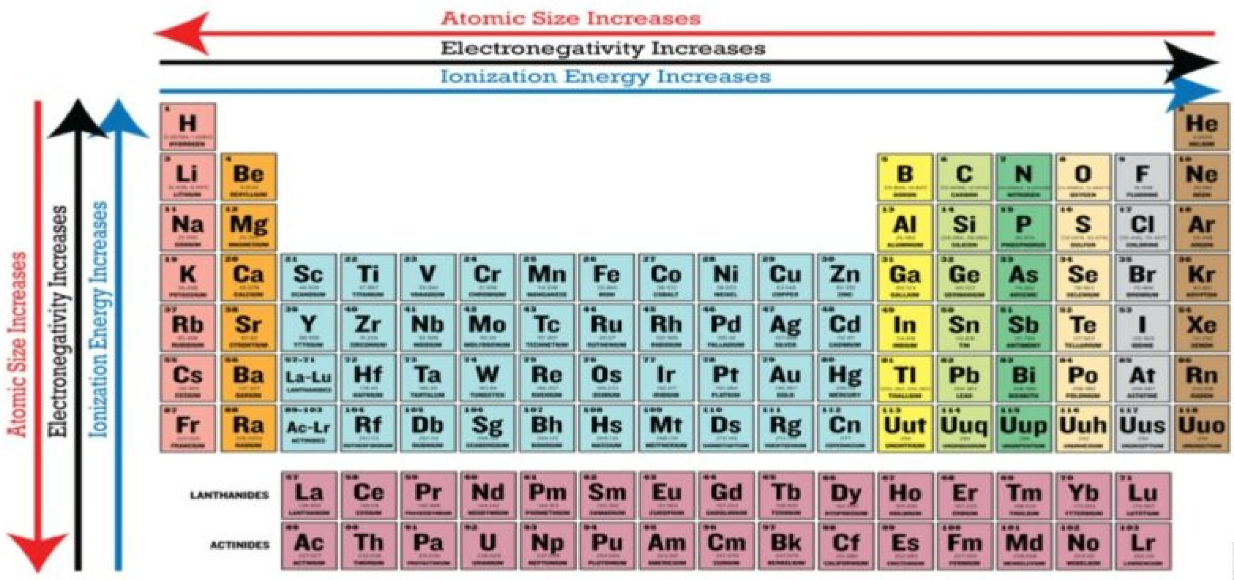

Fig-8: Trend of Atomic properties

Ionization Energy

- the energy necessary to remove an electron to form a positive ion
- low value for metals, electrons easily removed
- high value for non-metals, electrons difficult to remove
- increases from the lower-left corner of the periodic table to the upper right corner

Electron Affinity

- the energy released when an electron is added to an atom
- same trends as ionization energy increase from the lower-left corner to the upper right corner
- metals have low “EA”
- nonmetals have high “EA”

Quantum numbers

Principal quantum number, n

Principal quantum number tells the size of an orbital and largely determines its energy.

n= 1, 2, 3,..........

Angular momentum, l

Angular momentum exhibits the number of subshells that a principal level contains and it tells the shape of the orbitals.

l=0 to n-1

Magnetic quantum number, m1

The magnetic quantum number describes the direction that the orbital projects in space.

m1 = l to +1 (all integers, including zero)

For example, if l=2, then m1 would have values of -2, -1, 0, 1, and 2.

Knowing all the three quantum numbers provide us with a picture of all of the orbitals (**Table-3**).

Orbitals

Orbitals mean the region of the probability of finding an electron around the nucleus. There are four types of orbitals are available such as S, P, D, and F (**Fig-11 to 14**)

shell	n	l	m_l	type
K	1	0	0	1s
L	2	0 1	0 -1 0 1	2s 2p
M	3	0 1 2	0 -1 0 1 -2 -1 0 1 2	3s 3p 3d
N	4	0 1 2 3	0 -1 0 1 -2 -1 0 1 2 -3 -2 -1 0 1 2 3	4s 4p 4d 4f
O	5	0 1 2 3	0 -1 0 1 -2 -1 0 1 2 -3 -2 -1 0 1 2 3	5s 5p 5d 5f
P	6	0 1 2	0 -1 0 1 -2 -1 0 1 2	6s 6p 6d
Q	7	0	0	7s

Table: Quantum numbers

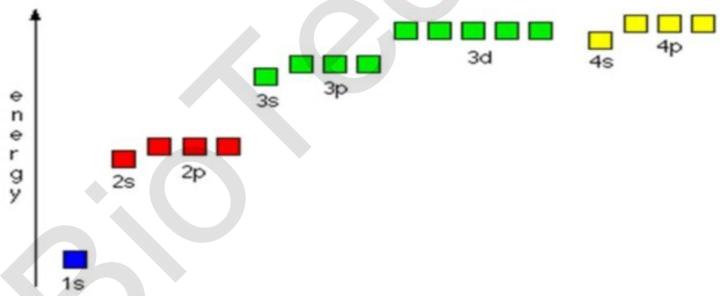

Fig-11: Orbital types

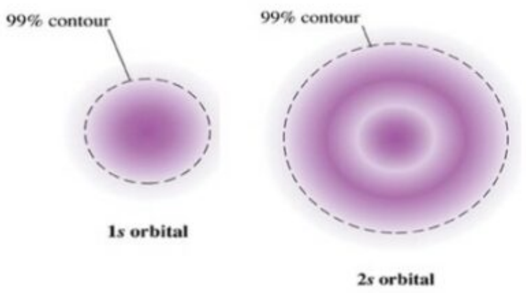

Fig-12: Atomic Orbitals, s-type

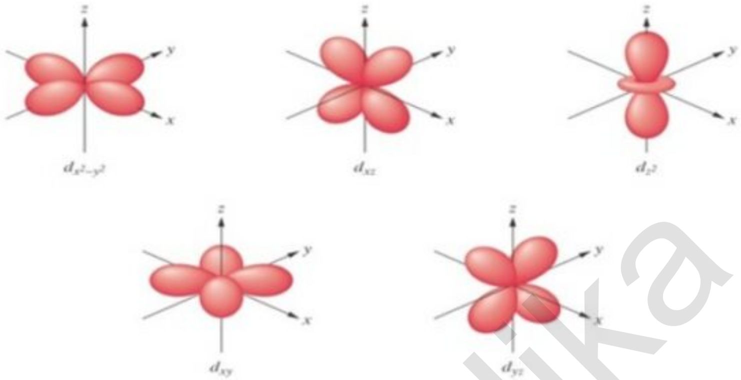

Fig-13: Atomic Orbitals, d-type

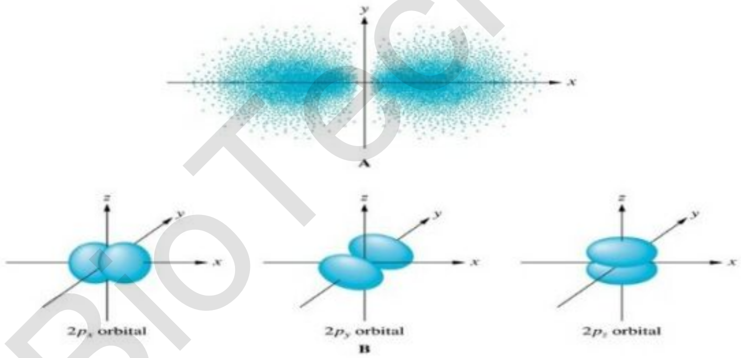

Fig-14: Atomic Orbitals, p-type

Electronic Configurations

The electronic configuration is the shorthand representation of the occupancy of the energy levels (shells and subshells) of an atom by electrons.

Electronic configuration can be represented in few ways as follows:

Example:

H atom (1 electron) – 1s1

He atom (2 electrons) – 1s2

Li atom (3 electrons) -1s2, 2s1

Cl atom (17 electrons) -1s2, 2s2, 2p6, 3s2, 3p5

As atom (33 electrons) – 1s2, 2s2, 2p6, 3s2, 3p6, 4s2, 3d10, 4p5

O – 1s2 2s2 2p4

Ti – 1s2 2s2 2p6 3s2 3p6 3d2 4s2

Br – 1s2 2s2 2p6 3s2 3p6 3d10 4s2 4p5

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Core format

O – [He] 2s2 2p4

Ti – [Ar] 3d2 4s2

Br – [Ar] 3d10 4s2 4p6

Electronic configuration of ions

Negative ions: **add electron(s), 1 electron for each negative charge**

S-2 ion: (16 + 2)electrons:

1s2, 2s2, 2p6, 3s2, 3p6

Positive ions **remove electron(s), 1 electron for each positive charge**

Mg+2 ion: (12-2) electrons

1s2, 2s2, 2p6

Chemical properties and the periodic table

Electron configurations help us understand changes in atomic radii, ionization energies, and electron affinities. Various trends in reactivity of periodic table elements can be observed. Main group metals become more reactive as you go down a group. The reactivity of nonmetals decreases as you go down a group. Transition metals become less reactive as you go down a group.

Hydrogen

Hydrogen is nonmetal under normal conditions. While it may lose an electron to form H+, it also can gain an electron to form H–. Hydrogen is commonly placed either in the group IA (1) or in the 1A(1) and VIIA(17) or not in any group.

Noble gases

Each of these has filled s and p sublevels except for helium (s only). All are very unreactive. A limited number of compounds have been produced using xenon and krypton. Noble gases are noted for their chemical stability and existence as monatomic molecules. Except for helium they share a common electron configuration that is very stable. This configuration has 8 valence-shell electrons.

Table: Noble gas configuration

Noble gas	Valence electron
He	2
Ne	8
Ar	8
Kr	8
Xe	8
Rn	8

Alkali metals

The group IA (1) metals all have an outer electron configuration of ns1. The loss of an electron to form a 1+ ion is the basis of almost all reactions of the alkali metals. This reactivity of the elements increases from top to bottom of the group.

Halogens

The common group VIIA (17) elements are all non-metals. Each only needs a single electron to achieve a noble gas configuration. When reacting with metals, they form 1- ions. When reacting with non-metals, they share electrons.

Lewis symbols

Represent the number of valence electrons as dots. The valence number is the same as the Periodic Table Group Number.

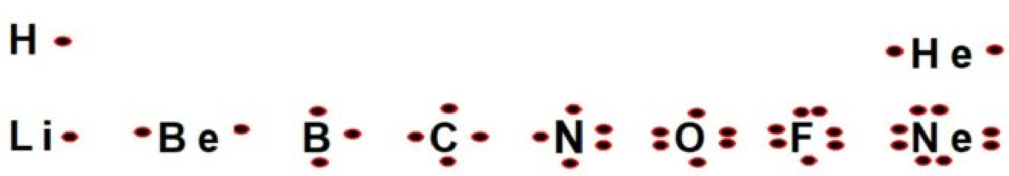

Fig: Lewis structure

The octet rule states that elements want to achieve the stable electron configuration of the nearest noble gas. Atoms tend to gain, lose or share electrons until they are surrounded by 8 electrons.

Resonance

Resonance occurs when more than one valid Lewis structure can be written for a particular molecule i.e. rearrange electrons.

Radical

Molecules and atoms which are neutral (contain no formal charge) and with an unpaired electron are called Radicals. A radical (more precisely, a free radical) is an atom, molecule, or ion that has unpaired valence electrons. With some exceptions, these unpaired electrons make free radicals highly chemically reactive toward other substances, or even towards themselves: their molecules will often spontaneously dimerize or polymerize if they come in contact with each other.

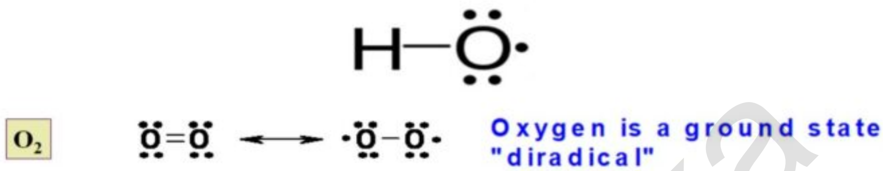

Fig: Radicals

VSEPR Model

VSEPR means Valence Shell Electron-Pair Repulsion. The structure around a given atom is determined principally by minimizing electron pair repulsions.

Valence shell electron pair repulsion theory states that in molecules there are 2 types of electrons.

1. Bonding Pairs
2. Non-bonding or lone pairs

The combinations of these electrons determine the shape of the molecule. Single bonds have a big impact on the shape, double bonds have little effect. The outer pairs of electrons around a covalently bonded atom minimize repulsions between them by moving as far apart as possible. CSIR NET UNIT 1 Notes by Biotecnika – FREE PDF Download.

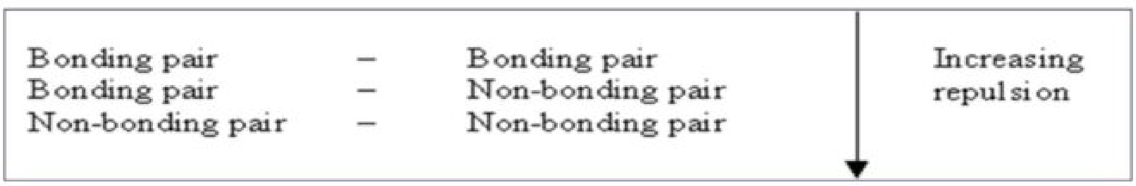

Fig: VSEPR Model postulates

Types of Bonds

Sigma Bonds

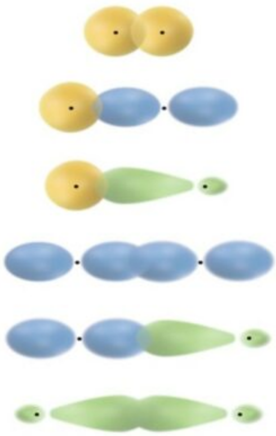

Fig: Sigma bond

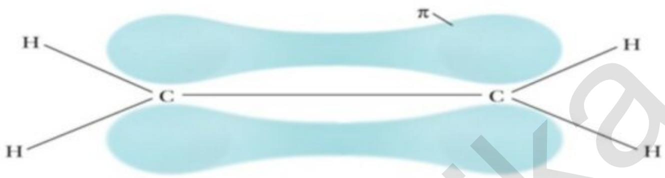

Fig: Pi-bond

Sigma bonds (s) mean the shared pair of electrons is symmetric about the line joining the two nuclei of the bonded atoms

Pi Bonds

Pi bonds (p) place electron density above and below the line joining the bonded atoms – they form by sideways overlap of *p* orbitals

Bonding in C2H4

The C-C sigma bond in C2H4 arises from the overlap of *sp2* hybrid orbitals and the four C-H sigma bonds from the overlap of *sp2* hybrid orbitals on C with 1*s* orbitals on H.The second C-C bond forms from the sideways overlap of *p* orbitals. The double bond in C2H4 is one sigma bond and one pi bond each bond is of similar strength.

Group 1 metals always form 1+ cations. Group 2 metals always form 2+ cations. Aluminum in Group 3 always forms a 3+ cation. Group 7 nonmetals form 1– anions.

Electron Configurations of Ions

Representative (main-group) metals form ions by losing enough electrons to achieve the configuration of the previous noble gas. Nonmetals form ions by gaining enough electrons to achieve the configuration of the next noble gas.

When a nonmetal and a Group 1, 2, or 3 metal react to form a binary ionic compound, the ions form so that the valence-electron configuration of the nonmetal achieves the electron configuration of the next noble gas atom. The valence orbitals of the metal are emptied to achieve the configuration of the previous noble gas. When two nonmetals react to form a covalent bond, they share electrons in a way that completes the valence-electron configurations of both atoms.

Predicting Formulas of Ionic Compounds

Chemical compounds are always electrically neutral.

Group 1	Group 2	Group 3	Group 6	Group 7	Electron Configuration
Li^+	Be^{2+}				[He]
Na^+	Mg^{2+}	Al^{3+}	O^{2-}	F^-	[Ne]
K^+	Ca^{2+}		S^{2-}	Cl^-	[Ar]
Rb^+	Sr^{2+}		Se^{2-}	Br^-	[Kr]
Cs^+	Ba^{2+}		Te^{2-}	I^-	[Xe]

Table: Common ions with Noble gas configurations in ionic compounds

Chemical Bonding

Chemical bonding is the force that holds the atoms together within a molecule (group of atoms of the same or different elements which exist together as a group)

A bond will form if the energy of the aggregate is lower than that of the separated atoms. Bond energy is the energy required to break a chemical bond.

Earlier theories of bonding

Lewis electronic theory

Lewis's electronic theory states that bonds are held together only by strong electrostatic forces of attraction. This theory couldn't explain many things like the formation of covalent bonds, stability of bonds, the exact shape of molecules, the existence of BF3 molecules, and the paramagnetic nature of oxygen atoms. Covalent bond was explained by valence bond theory and molecular orbital theory. CSIR NET UNIT 1 Notes by Biotecnika – FREE PDF Download.

Valence bond theory

Valence bond theory states that the covalent bond is formed by the overlap of the half-filled orbital. The two half-filled orbitals taking part in bond formation should have electrons with opposite spins. The direction of the bond is the same as the direction of overlap of the half-filled atomic orbitals. The valency of an element is the same as the number of half-filled orbitals. The strength of bonds depends upon the extent of overlap.

Molecular orbital theory

The molecular orbital theory states that when two atomic orbitals combine or overlap, they lose their identity and form a new orbital called molecular orbitals. Molecular orbitals are the energy state of a molecule in which the electrons of the atom are filled. A molecular orbital gives the electron probability distribution around a group of nuclei. Only those atomic orbitals will combine which have comparable energy. The number of molecular orbitals is equal to the number of combining orbitals. When two atomic orbitals combine they form two new orbitals called bonding orbital and antibonding orbital. The energy of bonding molecular orbital is less than the energy of the antibonding molecular orbital. The shape of the molecular orbital depends upon the shape of combining atomic orbital.

Mechanism of Bonding

The electrons which are involved in the bond are held together by the nuclei of each other. Lowering of energy takes place. Definite bond lengths and bond angles are formed.

Chemical Bonds

Chemical bonds are attractive forces that hold atoms together, thereby making molecules.

Types of Chemical Bonds

Covalent

- Polar
- Non-Polar

Non-Covalent

- Ionic Bonds
- Hydrogen Bonds
- Hydrophobic Interactions
- Van der Waals Forces

Ionic Bonds

Ionic bonds are formed by the complete transfer of electrons. Elements losing electrons are cations. Elements gaining electrons are anions. Electrostatic attraction between positively charged and negatively charged ions. The strength of ionic bonds in a cell is generally weak (**about 3 kcal/mol**) due to the presence of water, but deep within the core of a protein where water is often excluded such bonds can be much stronger.

Coordinate Bond

A coordinate bond is a type of bond where the two electrons involved in bonding are given by one species. It is also called a dipolar bond or dative covalent bond.

Eg: NH_3, chlorophyll, Haemoglobin

Van der Waals Forces

Van der waals forces are intermolecular forces. Van der Waals forces are weak forces because of dipole-dipole interaction, ion-dipole interaction, ion-induced dipole interaction, dipole induced dipole interaction, dispersion forces, and hydrogen bonding.

Dipole moment (μ)

Dipole moment (μ) is the product of the magnitude of the separated charge and the distance of the separation. It is a quantity that describes two opposite charges by a distance. It is a quantity that we can measure for a molecule in the lab and thereby determine the size of partial charges on the molecule (If we know the bond length)

Dipole moment representation

Property of a molecule whose charge distribution can be represented by a center of positive charge and a center of negative charge. Use an arrow to represent a dipole moment. Point to the negative charge center with the tail of the arrow indicating the positive center of the charge.

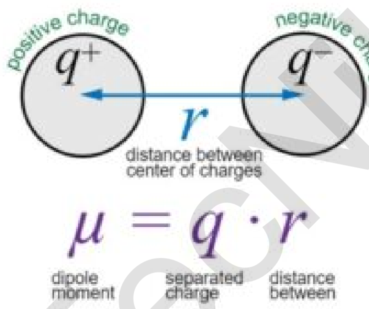

Fig : Dipole moment (where q is the magnitude of the separated charge and r is the distance between them)

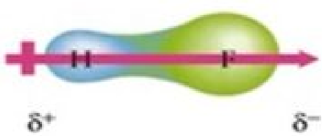

Fig : Dipole moment representation

Dipole-dipole interaction

Dipole-dipole interaction occurs among polar groups. Polar molecules have permanent dipoles. One positive pole and one negative pole. A positive pole attracts a negative pole.

Ion-dipole interaction

In Ion-dipole interaction, the attraction will occur between an ion and a polar molecule. The strength of the interaction depends upon the charge, size of the ion, magnitude of dipole moment, and size of the polar molecule. Interaction is stronger in the case of cation as cation has more charge density and small size.

Ion-induced dipole interaction

Ion-induced dipole interaction occurs between non-polar molecules and ions. After the interaction, a non-polar molecule is induced to become polar. Here the strength of the interaction depends on the charge of the ion. CSIR NET UNIT 1 Notes by Biotecnika – FREE PDF Download.

Dipole induced dipole interaction

Dipole-induced dipole interaction occurs between a polar and a nonpolar molecule. A polar molecule when it reacts with the nonpolar molecule, it will make the nonpolar become polar. The strength of this interaction depends upon the strength of the dipole and the ease of the polarizability of the nonpolar molecule.

London forces or Dispersion forces

London forces were proposed by Fritz London in 1930. London force arises from the motion of electrons. Electron cloud when distorted produces instantaneous dipole or momentary dipole which induces a dipole in neighboring molecules. The magnitude of the force depends on the complexity and geometry of molecules.

Bond Length

Distances between centers of bonded atoms are called bond lengths or bond distances.

Bond Strength

The amount of energy required to break a bond is called bond dissociation energy or simple bond energy.

Ionic Bonding

Ionic compound results when a metal reacts with a nonmetal and electrons are transferred

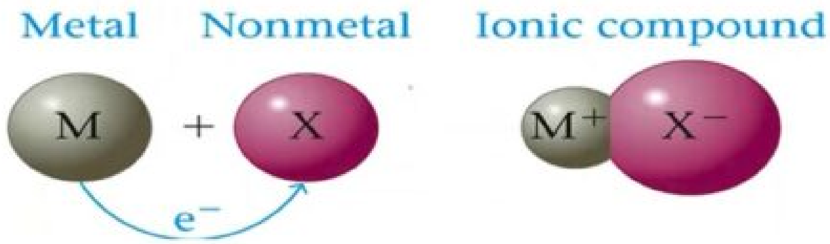

Fig: Ionic bonding

Ionic bonds are formed by the attraction of oppositely charged ions

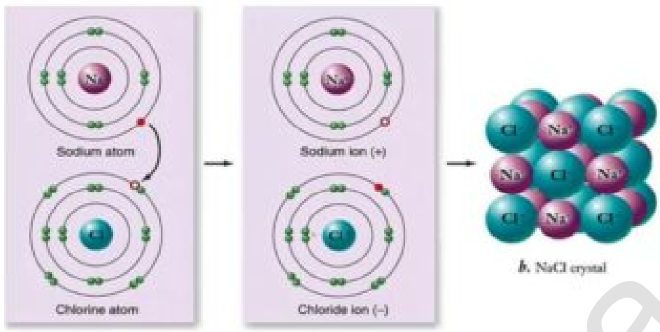

Fig: Ionic bond formation in Nacl

Metals have a tendency to lose electrons to form cations. Nonmetal gains electrons to form an anion. The electronegativity between the metal and nonmetal must be greater than 2. Ionic bond results from positive to negative attraction. The ionic bond will have stronger attraction if the element will have a larger charge and smaller ion. Lewis's theory allows us to predict the correct formulas of ionic compounds.

Ionic substances are formed when an atom that loses electrons relatively easily reacts with an atom that has a high affinity for electrons. **Eg**: metal-nonmetal compound.

Structures of Ionic compounds

Ions are packed together to maximize the attraction between ions.

Isoelectronic series

A series of ions/atoms containing the same number of electrons. **Eg**: O^{2-}, F^{-}, Ne, Mg^{2+}, and Al^{3+}

Covalent Bonding

A covalent bond results when electrons are shared by nuclei. An electron density plot for the H_2 molecules shows that the shared electrons occupy a volume equally distributed over both hydrogen atoms.

Most of the molecules in living systems contain only six different atoms: hydrogen, carbon, nitrogen, phosphorus, oxygen, and sulfur. These atoms readily form covalent bonds with other atoms and rarely exist as isolated entities. As a rule, each type of atom forms a characteristic number of covalent bonds with other atoms. Covalent bonds tend to be very stable because the energies required to break or rearrange them are much greater than the thermal energy available at room temperature (25°C) or body temperature (37°C). Covalent bonds are often found between two nonmetals. Atoms bonded together to form molecules and have a strong attraction. Atoms share a pair of electrons to attain octets. CSIR NET UNIT 1 Notes by Biotecnika – FREE PDF Download.

In a covalent bond shared electrons are attracted to the nuclei of both atoms. They move back and forth between the outer energy levels of each atom in a covalent bond. So, each atom has a stable outer energy level some of the time.

Polar Covalent Bond

Unequal sharing of electrons between atoms in a molecule. One atom attracts the electrons more than the other atom. Results in a charge separation in the bond (partial positive and partial negative charge). Eg: HF

The polarity of a bond depends on the difference between the electronegativity values of the atoms forming the bond

Single Covalent Bond

Two atoms share one pair of electrons (2 electrons). One atom may have more than one single bond. Single covalent bonds compounds are less reactive and have a high bond length. It was denoted by Single dash. **Eg**: Fluorine molecules, water

Double covalent bond

Double covalent bonds are formed by sharing two pairs of valence electrons. The double covalent bond compound was moderately reactive and has a moderate bond length. It was denoted by two parallel dashes.

Triple covalent bond

Triple covalent bonds are formed by sharing three pairs of valence electrons. The triple covalent bond compound was highly reactive and has a low bond length. It was denoted by three parallel dashes.