

Points to Remember

Class: XI

Chapter Name: Chemical Bonding and Molecular Structure

Top Concepts

1. The attractive force which holds together the constituent particles (atoms, ions or molecules) in chemical species is known as chemical bond.
2. Tendency or urge atoms of various elements to attain stable configuration of eight electrons in their valence shell is cause of chemical combination.
3. The principle of attaining a maximum of eight electrons in the valence shell or outermost shell of atoms is known as octet rule.
4. Electronic Theory: Kossel-Lewis approach to chemical Bonding: Atoms achieve stable octet when they are linked by chemical bonds. The atoms do so either by transfer or sharing of valence electrons. Inner shell electrons are not involved in combination process.
5. Lewis Symbols or electron dot symbols: The symbol of the element represents the whole of the atom except the valence electrons (i.e. nucleus and the electrons in the linear energy shells). The valence electrons are represented by placing dots (.) or crosses (x) around the symbol.
6. Significance of Lewis Symbols: The Lewis symbols indicate the number of electrons in the outermost or valence shell which helps to calculate common or group valence.
7. The common valence of an element is either equal to number of dots or valence electrons in the Lewis symbol or it is equal to 8 minus the number of dots or valence electrons.
8. The bond formed by mutual sharing of electrons between the combining atoms of the same or different elements is called a covalent bond.
9. If two atoms share one electron pair, bond is known as single covalent bond and is represented by one dash (-).

10. If two atoms share two electron pairs, bond is known as double covalent bond and is represented by two dashes (=)

11. If two atoms share three electron pairs, bond is known as triple covalent bond and is represented by three dashes (\equiv).

12. The formal charge of an atom in a polyatomic ion or molecule is defined as the difference between the number of valence electrons in an isolated (or free) atom and the number of electrons assigned to that atom in a Lewis structure. It may be expressed as:

Formal charge
on an atom =
in free atom

$$\left(\begin{array}{l} \text{Number of} \\ \text{valence electrons} \\ \text{in free atom} \end{array} \right) - \left(\begin{array}{l} \text{Number of} \\ \text{nonbonding} \\ \text{(lone pair) electrons} \end{array} \right) - \frac{1}{2} \left(\begin{array}{l} \text{Number of} \\ \text{bonding} \\ \text{(shared) electrons} \end{array} \right)$$

13. Significance of Formal charge: The formal charges help in selection of lowest energy structure from a number of possible Lewis structures for a given molecule or ion. Lowest energy structure is the one which has lowest formal charges on the atoms.

14. Expanded octet: Compounds in which central atom has more than eight electrons around it, atom is said to possess an expanded octet.

15. Exceptions to the Octet Rule:

Hydrogen molecule: Hydrogen has one electron in its first energy shell ($n = 1$). It needs only one more electron to fill this shell, because the first shell cannot have more than two electrons. This configuration ($1s^2$) is similar to that of noble gas helium and is stable. In this case, therefore, octet is not needed to achieve a stable configuration.

Incomplete octet of the central atom: The octet rule cannot explain the formation of certain molecules of lithium, beryllium, boron, aluminum, etc.

(LiCl, BeH₂, BeCl₂, BH₃, BF₃) in which the central atom has less than eight electrons in the valence shell as shown below:

Expanded octet of the central atom: There are many stable molecules which have more than eight electrons in their valence shells. For example, PF₅, has ten; SF₆ has twelve and IF₇ has fourteen electrons around the central atoms, P, S, and I respectively.

Odd electron molecules: There are certain molecules which have odd number of electrons, like nitric oxide, NO and Nitrogen dioxide, NO₂. In these cases, octet rule is not satisfied for all the atoms.

It may be noted that the octet rule is based upon the chemical inertness of noble gases. However, it has been found that some noble gases (especially xenon and krypton) also combine with oxygen and fluorine to form a large number of compounds such as XeF₂, KrF₂, XeOF₂, XeOF₄, XeF₆, etc.

This theory does not account for the shape of the molecules.

It cannot explain the relative stability of the molecule in terms of the energy.

16. General Properties of Covalent Compounds

1. The covalent compounds do not exist as ions but they exist as molecules.
2. The melting and boiling points of covalent compounds are generally low.
3. Covalent compounds are generally insoluble or less soluble in water and other polar solvents. However, these are soluble in non-polar solvents.
4. Since covalent compounds do not give ions in solution, these are poor conductors of electricity in the fused or dissolved state.

5. Molecular reactions are quite slow because energy is required to break covalent bonds.

6. Since the covalent bond is localized in between the nuclei of atoms, it is directional in nature.

17. Co- Ordinate Covalent Bond:

Covalent type bond in which both the electrons in the shared pair come from one atom is called a coordinate covalent bond.

Co- Ordinate Covalent Bond is usually represented by an arrow (\rightarrow) pointing from donor to the acceptor atom.

Co- Ordinate Covalent bond is also called as dative bond, donor – acceptor bond, semi- polar bond or co-ionic bond.

18. The electrostatic force of attraction which holds the oppositely charged ions together is known as ionic bond or electrovalent bond.

19. Ionic compounds will be formed more easily between the elements with comparatively low ionization enthalpy and elements with comparatively high negative value of electron gain enthalpy.

20. A quantitative measure of the stability of an ionic compound is provided by its lattice enthalpy and not simply by achieving octet of electrons around the ionic species in the gaseous state

21. Lattice enthalpy may also be defined as the energy required to completely separating one mole of a solid ionic compound into gaseous ionic constituents.

22. Factor affecting lattice enthalpy:

Size of the ions: Smaller the size of the ions, lesser is the internuclear distance and higher will be lattice enthalpy.

Larger the magnitude of charge on the ions, greater will be the attractive forces between the ions. Consequently, the lattice enthalpy will be high.

23. General Properties of Ionic Compounds

Ionic compounds usually exist in the form of crystalline solids.

Ionic compounds have high melting and boiling points.

Ionic compounds are generally soluble in water and other polar solvents having high dielectric constants.

Ionic compounds are good conductors of electricity in the solutions or in their molten states.

The chemical reactions of ionic compounds are characteristic of the constituent ions and are known as ionic reactions.

In ionic – compounds, each ion is surrounded by oppositely charged ions uniformly distributed all around the ion and therefore, electrical field is non-directional.

24. Bond length: It is defined as the average distance between the nuclei of the nuclei of two bonded atoms in a molecule.

25. Covalent radius is half of the distance between two similar atoms joined by single covalent bond in same molecule.

26. Van der Waals radius is one half of the distance between two similar adjacent atoms belonging to two nearest neighbouring molecules of the same substance in the solid state. It is always larger than covalent radii.

27. Bond angle: It is defined as the average angle between orbitals containing bonding electron pairs around the central atom in a molecule.

28. Bond enthalpy: It is defined as amount of energy required to break one mole of bonds of a particular type between atoms in gaseous state.

29. Bond order: The bond order is defined as the number of bonds between two atoms in a molecule.
30. When a single Lewis structure cannot determine a molecule accurately, concept of resonance is used wherein a number of structures with similar energy, positions of nuclei, bonding and non-bonding pairs of electrons are taken as canonical structures of hybrid which describes molecule accurately.
31. Resonance: When a molecule cannot be represented by a single structure but its characteristic properties can be described by two or more than two structures, then the actual structure is said to be a resonance hybrid of these structure.
32. Polarity of Bonds: In reality no bond is completely covalent or completely ionic.
33. Non-polar covalent bond: When a covalent bond is formed between two similar atoms, the shared pair of electrons is equally attracted by the two atoms and is placed exactly in between identical nuclei. Such a bond is called non-polar covalent bond
34. Molecules having two oppositely charged poles are called polar molecules and the bond is said to be polar covalent bond. Greater the difference in the electro-negativity of the atoms forming the bond, greater will be the charge separation and hence greater will be the polarity of the molecule.
35. Dipole moment is defined as the product of the magnitude of the charge and the distance of separation between the charges.
- Dipole moment (μ) = charge (q) x distance of separation (d)
36. Partial Covalent Character in Ionic Bonds: When two oppositely charge ions A^+ and B^- are brought together; the positive ion attracts the outermost electrons of the negative ion. This results in distortion of

electron clouds around the anion towards the cation. This distortion of electron cloud of the negative ion by the positive ion is called polarization.

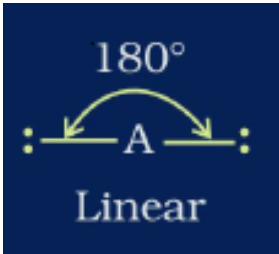
37. Tendency of cation to polarize and polarisability of anion are summarized as Fajan's rules:


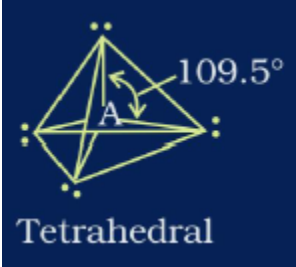


- a. Smaller the size of the cation, greater is its polarizing power.
- b. Polarisation increases with increase in size of anion. This is because the electron cloud on the bigger anion will be held less firmly by its nucleus and, therefore, would be more easily deformed towards the cation.
- c. Larger the charge on cation greater is polarizing power and larger the charge on anion greater is its tendency to get polarized.

38. Valence Shell Electron Pair Repulsion (VSEPR) Theory:

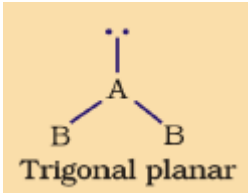
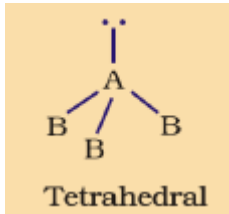
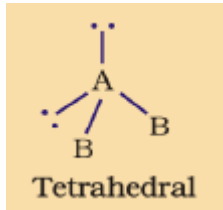
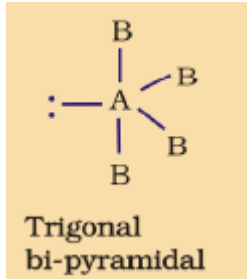
Since Lewis symbols were unable to explain shapes of certain molecules, VSEPR theory was introduced. The basic idea of this theory is that bonded atoms in a molecule adopt that particular arrangement in space around the central atom which keeps them on the average as far apart as possible.

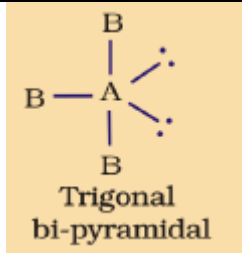
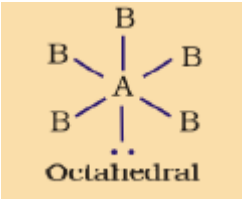
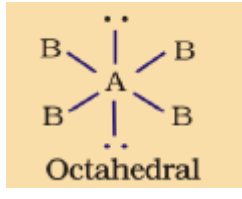
39. Geometry and shapes of molecules in which central atom has no lone pair of electrons

Number of electron pairs	Arrangement of electron pairs	Molecular geometry	Examples
2		Linear	BeCl ₂ , HgCl ₂

3		Trigonal planar	BF ₃
4		Tetrahedral	CH ₄ , NH ₄ ⁺
5		Trigonal bipyramidal	PCl ₅
6		Octahedral	SF ₆

Shapes of simple molecules/Ions with central ions having one or more lone pairs of electrons

Molecule type	No. of bonding pairs	No. of lone pairs	Arrangement of electron pairs	Shape	Example
AB_2E	2	1	 <p>Trigonal planar</p>	Bent	SO_2, O_3
AB_3E	3	1	 <p>Tetrahedral</p>	Trigonal pyramidal	NH_3
AB_2E_2	2	2	 <p>Tetrahedral</p>	Bent	H_2O
AB_4E	4	1	 <p>Trigonal bi-pyramidal</p>	See saw	SF_4

AB_3E_2	3	2	 <p>Trigonal bi-pyramidal</p>	T-shape	ClF_3
AB_5E	5	1	 <p>Octahedral</p>	Square pyramidal	BrF_5
AB_4E_2	4	2	 <p>Octahedral</p>	Square planar	XeF_4

A: Central atom, B is surrounding atoms, E is the lone pair

40. Valence Bond Approach of Covalent Bond

The VSEPR theory gives the geometry of simple molecules but theoretically, it does not explain them and also has limited applications. To overcome these limitations, two important theories based on quantum mechanical principles are commonly used. These are Valence bond (VB) theory and Molecular orbital (MO) theory.

41. Valence Bond Theory

- A discussion of valence bond theory is based on the knowledge of atomic orbitals, electronic configuration of elements, overlap criteria of atomic orbitals and principles of variation and superposition.
- Orbital Overlap Concept of Covalent Bond: When two atoms approach each other, partial merger of two bonding orbitals, known as overlapping of the orbitals occurs.

- Depending upon the type of overlapping, the covalent bonds may be divided as sigma (σ) bond and Pi (π) bond.
- Sigma (σ) bond: This type of covalent bond is formed by the end to end (hand on) overlapping of bonding orbitals along the inter-nuclear axis. The overlap is known as head on overlap or axial overlap. The sigma bond is formed by any one of the following types of combinations of atomic orbitals. Sigma (σ) bond can be formed by $s - s$ overlapping, $s - p$ overlapping, $p - p$ Overlapping etc.
- Pi (π) Bond: This type of covalent bond is formed by the sidewise overlap of the half- filled atomic orbitals of bonding atoms. Such an overlap is known as sidewise or lateral overlap.

42. Hybridization:

- In order to explain characteristic geometrical shapes of polyatomic molecules concept of hybridization is used.
- The process of intermixing of the orbitals of slightly different energies so as to redistribute their energies resulting in the formation of new set of orbitals of equivalent energies and shape.

43. Atomic orbitals used in different types of hybridization.

Shapes of molecules/ions	Hybridisation type	Atomic orbitals	Examples
Linear	sp	one s + one p	BeCl_2
Trigonal planar	sp^2	one s + two p	BCl_3
Tetrahedral	sp^3	one s + three p	CH_4, NH_3
Square planar	dsp^2	one d + one s + two p	$[\text{Ni}(\text{CN})_4]^{2-}$ $[\text{Pt}(\text{Cl})_4]^{2-}$
Trigonal bipyramidal	sp^3d	one s + three p + one d	$\text{PF}_5, \text{PCl}_5$

bipyramidal			
Square pyramidal	sp^3d^2	one s +three p +two d	BrF_5
Octahedral	sp^3d^2 d^2sp^3	one s +three p +two d two d + one s +three p	$SF_6, [CrF_6]^{3-}, [Co(NH_3)_6]^{3+}$

44. Molecular Orbital Theory (MOT):

- Basic idea of MOT is that atomic orbitals of individual atoms combine to form molecular orbitals. Electrons in molecule are present in the molecular orbitals which are associated with several nuclei.
- The molecular orbital formed by the addition of atomic orbitals is called the bonding molecular orbital (σ).
- The molecular orbital formed by the subtraction of atomic orbital is called antibonding molecular orbital (σ^*).
- The sigma (σ) molecular orbitals are symmetrical around the bond-axis while pi (π) molecular orbitals are not symmetrical.
- Sequence of energy levels of molecular orbitals changes for diatomic molecules like $Li_2, Be_2, B_2, C_2, N_2$ is $\sigma 1s < \sigma^* 1s < \sigma 2s < \sigma^* 2s < (\pi 2p_x = \pi 2p_y) < \sigma 2p_z < (\pi^* 2p_x = \pi^* 2p_y) < \sigma^* 2p_z$
- Sequence of energy levels of molecular orbitals changes for diatomic molecules like O_2, F_2, Ne_2 is $\sigma 1s < \sigma^* 1s < \sigma 2s < \sigma^* 2s < \sigma 2p_z < (\pi 2p_x = \pi 2p_y) < (\pi^* 2p_x = \pi^* 2p_y) < \sigma^* 2p_z$

Bond order (b.o.) is defined as one half the difference between the number of electrons present in the bonding and the antibonding orbitals

45. Hydrogen Bonding:

- The attractive force which binds hydrogen atom of one molecule with electronegative atom like F, O or N of another molecule is known as hydrogen bond or hydrogen bonding.
- Magnitude of hydrogen bonding is maximum in solid state and least in gaseous state.

- Intermolecular hydrogen bond is formed between two different molecules of same or different substances.
- Intramolecular hydrogen bond is formed between the hydrogen atom and highly electronegative like O, F or N present in the same molecule.

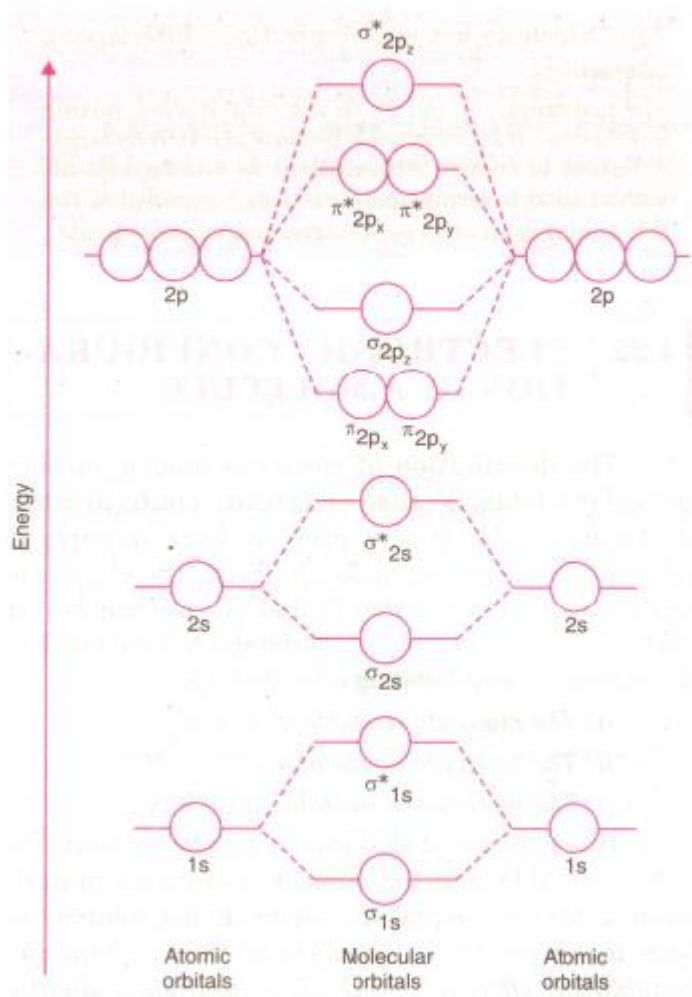
Top Formula:

1.

$$\% \text{ ionic character} = \frac{\text{Observed dipole moment}}{\text{Dipole moment for complete ionic character}} \times 100$$

Top Diagrams

Molecular orbital energy level diagram for Li_2 , Be_2 , B_2 , C_2 , N_2 molecules



Molecular orbital energy level diagram for O_2 , F_2 , Ne_2 etc.

