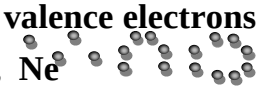
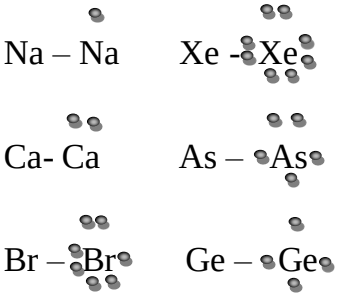
4	Chemical Bonding and Molecular Structure	Book: H.C. Srivastava

Q – 1 Very Short Question Answers.

1. **How many electrons are present in a sextet and in an octet ?**
   6, 8
2. **How many valence electrons do the atoms represented by following Lewis structures possess?**
   Li, B , O , Ne
   
   1, 3, 6, 8
3. **Draw the Lewis symbols of the following elements. Na, Ca, Br, Xe, As, Ge**
   

4. **Draw the Lewis structures for the following molecules and ions and tell which do not follow the octet rule. F_2, PH_3, H_2S, $SiCl_4$, C_3H_8, F_2O, Na^+, Cl^-**
   PH_3, H_2S, C_3H_8 do not follow octet rule.
5. **What type of force does exist between two atoms in anionic bond?**
   Electrostatic force of attraction.
6. **Short out the most and the least electronegative atoms among the following :**
   Cl, Na, O, N, S, F, Cs
   F, Cs
7. **What type of bonds are expected to be formed between atoms having electronegativity difference (i) equal to zero; (ii) equal to 1.1; (iii) equal to 2.0.**
   (i) Covalent (ii) Covalent (iii) Ionic.
8. **Which property of water is helpful in the dissolution of an ionic solid in it?**
   High dielectric constant
9. **Why are the noble gases monoatomic?**
   Due to stable electronic configuration they have no tendency to combine with each other.
10. **Define bond energy.**
    The amount of energy required to break one mole of bonds of the same kind to separate the bonded atoms in the gaseous state.
11. **Among NH_3 and PH_3 which is expected to have a higher dipole moment and why?**
    NH_3, due to higher electronegativity of N.
12. **Do van der Waals' forces exist between the atoms of noble gases?**
    Yes

13. What is octet rule?

During the formation of a molecule, an atom of a particular element gains, loses or shares electrons unit it acquire a stable electronic configuration of eight electrons in its valence shell.

14. What do you understand by lattice energy?

The amount of energy liberated in condensing the required number of cations and anions to form the lattice of one gram mole of an ionic compound is called the lattice energy of that compound.

15. The elements of which groups prefer to form cations?

Groups 1 and 2

16. Do elements of groups1 and 2 show variable electrovalency?

No

17. Do ionic solids conduct electric current in the solid state?

No

18. Define a covalent bond.

The attractive force which comes into existence due to the mutual sharing of electrons between two atoms of similar electronegativity or having small difference in electronegativity.

19. How many covalent bonds are present in a molecule of ethylene?

Six

20. Which of the following elements does not show variable covalency? Al, F, S, Cl

Al

21. What is the maximum covalency of sulphur?

Six

22. How many singlet linkages are present in the Sugden's structure of SF_6?

Four

23. When does a covalent bond acquire partial ionic character?

When a covalent bond is formed between two atoms of different electronegativities, the atom with a higher value of electronegativity tries to pull the shared pairs to a greater extent as compared to the atom with a value of lower electronegativity. The covalent bond thus developed a partial ionic character in it.

24. When does an ionic bond develop a partial covalent character?

When an ionic compound contains a small cation and a large anion, the positively charged cation attracts the outermost electrons of the anion and repels its positively charged nucleus. This results in the distortion or polarization of the anion followed by some sharing of electrons between the two. Consequently, the ionic bond acquires some covalent character.

25. Among AgCl and AgI, which is more covalent?

AgI

26. Can a π-bond be formed without the formation of a σ-bond?

No

27. What type of orbitals can overlap to form a covalent bond?

Half-filled orbital

28. What happens to the potential energy of the system when two atoms form a covalent bond?

Potential energy decreases

29. Is hybridization between the orbitals of two atoms possible?

No

30. What type of bond is formed when two ρ-orbitals overlap axially?

σ bond

31. How many σ and π bonds are present in CH_3-CH=CH_2?

Eight σ and one π bonds

32. How much s and ρ characters are present in sp^3 hybrid orbitals?

25% s and 75% p character.

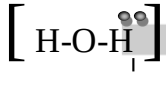
33. What type of hybridisation do you expect in the following molecules? BF_3, CH_4, C_5H_6, BeF_2.

BF_3-sp^2, CH_4-sp^3, C_6H_6-sp^2, BeF_2-sp.

34. In what respect a coordinate covalent bond is different from a covalent bond?

A coordinate covalent bond is a covalent bond in which both the electrons of the shared pair come from one of the two combining atoms.

35. Illustrate the formation of H_3O^+.



36. What is a kernel and how is it formed?

When an atom loses one or more of its valence electron, the remaining part of the atom left is called core or kernel.

37. Does the presence of intermolecular hydrogen bonding affect the boiling point of a liquid?

No, because it does not associate the molecules

38. Why are the molecular orbitals regarded as polycentric?

In a molecular orbital, the electron cloud is associated with the molecule as a whole and is spread over the whole nuclear system of the combining atoms. A molecular orbital is thus polycentric.

39. Among σ_{2s} and σ^*_{2s} molecular orbitals, which one is of lower energy?

σ_{2s}

40. If ψ_A and ψ_B are the wave functions of two combining hydrogen atoms, what would be the wave functions of bonding and antibonding molecular orbitals formed by their combination?

$\Psi_b = \psi_A + \psi_B$, $\psi_a = \psi_A - \psi_B$

41. What is the probability of finding electrons between the nuclei of the combining atoms in an antibonding molecular orbital?

Negligible

42. For a molecule, $N_b=N_a$, will the molecule be stable?

No

43. How is bond length related to the bond order of the molecule?

Bond length is inversely proportional to the bond order

44. The bond order of He^{2+} ion is 1/2. Comment on its magnetic nature.

Paramagnetic

45. What for does KK stand in the molecular orbital electronic configuration KK $(\sigma_{2s})^2$ for Li_2 molecule?

Closed K shell structure $(\sigma_{1s})^2$ $(\sigma^*_{1s})^2$.

46. According to the molecular orbital theory, how many unpaired electrons are present a O_2 molecule?

2

47. Carbon atom possesses only two unpaired electrons. How is it able to show tetracovalency?

48. What are the hybrid states of C atoms in alkanes, alkenes and alkynes?

sp^3, sp^2 and sp

Q – 2 Short question Answers.

1. **Why do atoms combine together and form molecules?**

   The theory of chemical bonding reveals that the formation of a chemical bonds involves a decrease in the potential energy of the system. So, atoms combine together and form molecules.

2. **What types of bonds will be formed between the following pairs of elements and why? (a) K, Cl (b) Ca, S (c) N, H (d) C, O**

   (a) Ionic (b) ionic (c) covalent (d) covalent; explain in terms of electronegativity.

3. **What is lattice energy and how is it related to the stability of anionic compound?**

   The amount of energy liberated in condensing the required number of cations and anions to form the lattice of one gram mole of an ionic compound.

   Higher the value of lattice energy, higher is the stability of compound.

4. **Define Electronegativity. How does it vary in the periodic table?**

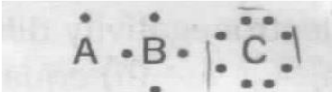
   The tendency of an atom to attract the bonding or shared paired electrons towards its own side in a covalent bond.

   It increases across a period. It decreases down a group.

5. **Deduce the empirical formula and draw the Lewis structures for the ionic compounds formed by the following pairs of elements. Na, O; K, S; Na, P; Mg, Br; Al, F; Ca, O; Li, S.**

   Na_2O, K_2S, Na_3P, $MgBr_2$, AlF_3, CaO, U_2S; write the Lewis structure on the basis of these formula.

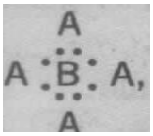
6. **Three elements have the following Lewis symbols.**

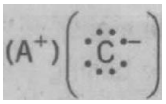


(i) Place the elements in the appropriate groups of the periodic table, (ii) Which elements are likely to form Jons? What is the expected charge on ions? (iii) Write the formula and the Lewis structures of the covalent compounds formed between (a) A and B, (b) A and C.

(i) Group 1, Group 14, Group 17

(ii) A and C will form ions -A^+, C^-

(iii) (a) BA_4; 

(b) AC; 

7. **Explain why ionic compounds (i) possess high melting and boiling points; (ii) are soluble in water; (iii) are hard and brittle.**

(i) It is because in an ionic compound, the oppositely charged ions are tightly held together in their specific position by strong electrostatic forces. It requires a high temperature to overcome these forces.

(ii) Ionic compounds are soluble in water because water has a high dielectric constant and weakers the electrostatic force of attraction existing between the ions. The ions thus get separated and get surrounded by water molecules

(iii) The ionic compounds are hard and brittle because the strong electrostatic force exists between the ions.

8. **Why do covalent compounds exhibit stereoisomerism?**

The covalent bonds are rigid and directional. These bonds are formed by the sharing of electrons and remain directed in specific directions in space. So, covalent compounds exibit stereoisomerism.

9. **What do you understand by bond length? On what factors does it depend?**

The average distance between the centres of the nuclei of two bonded atoms in a molecule.

The factors on which it depend are :

(i) Size of atom : Bond length increases with the increase in atomic size.

(ii) Multiplicity of bond : Bond length decreases with the increase in multiplicity of bonds.

10. **Carbon possesses only two unpaired electrons in its valence shell. How does it show a covalency equal to four in most of its compounds?**

Carbon possess only two unpaired electrons in its valence shell but exibit a covalency of 4 because in excited state the paired electron from 2s subshell migrates to $2p_z$ subshell which leads to 4 unpaired electrons.

11. **Why does a covalent bond develop a partial ionic character when the electronegativities of the combining atoms are different?**

A covalent bond develops a partial ionic character when the electronegativities of combining atoms are different because the element with higher electronegativity will pull the electrons towards itself which results in development of partial –ve charge and partial +ve charge on other.

12. You are given five neutral atoms A, B, C, D and E having the following electronic configuration : A-$1s^2 2s^2 2p^6 3s^2$, D-$1s^2 2s^2 2p^5$, B-$1s^2 2s^2 2p^6 3s^1$, E-$1s^2 2s^2 2p^6$, C-$1s^2 2s^2 2p^1$ Write the empirical formula for the substances containing : (i) A and D (ii) B and D (iii) only D (iv) only E.

(i) AD_2 (ii) BD (iii) D_2 (iv) E (monoatomic)

13. Why is ionic bond regarded as an extreme case of a polar covalent bond?

The ionic species with opposite charge are formed which are held by electrostatic forces of attraction rather situation is almost equivalent to the complete transfer of electron from the less electronegative atom as happens during the formation of an ionic bond. Thus, an ionic bond is regarded as external case of polar covalent bond.

14. Define bond energy. On what factors does it depend?

The amount of energy required to break one mole of bond of same kind to separate the bonded atoms in gaseous state.

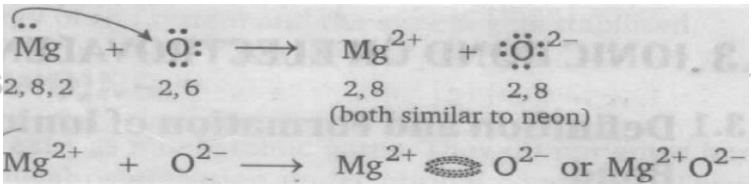
The factors are :

(i) Size of atoms : Bond energy decrease with increase in size of atoms.

(ii) Multiplicity of bonds : Bond energy increases with increase in multiplicity of bonds.

15. Discuss the formation of MgO.

The electronic configuration of magnesium is $1s^2\ 2s^2\ 2p^6\ 3s^2$ (2, 8, 2), while that of oxygen is $1s^2\ 2s^2\ 2p^4$ (2, 6). Magnesium being an electropositive element loses its two valence electrons to attain the stable electronic configuration of its nearest inert gas Ne (2, 8), whereas oxygen gains these electrons to attain the stable configuration similar to that of Ne. Thus, magnesium changes into Mg^{2+} ion and oxygen into O^{2-} ion. The two ions get linked together by strong electrostatic force of attraction. Thus, MgO molecule is formed as shown below



16. Discuss the factors which govern the formation of an ionic bond.

The factors are :

(i) Low value of ionization energy

(ii) More negative value of electronegative atom

(iii) The difference of electronegativities between two atoms in more than 2.

17. What do you understand by variable electrovalency? Give some examples.

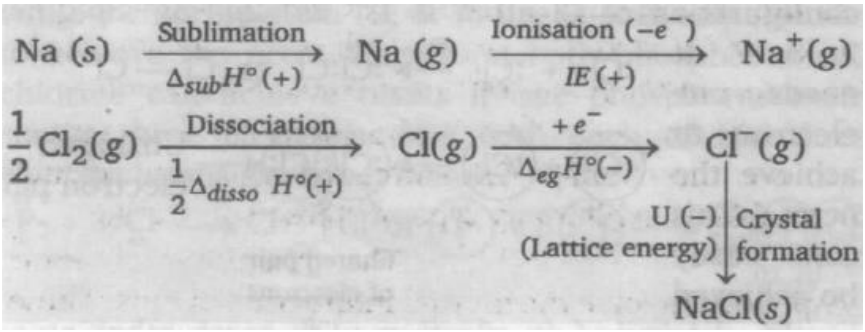
The atom which are capable of showing more than one type of ions having different charges. This is the phenomenon. Eg. Cuprous : Cu^+, Cupric : Cu^{2+} and Ferrous : Fe^{2+}, Ferric : Fe^{3+}

18. What is inert pair effect? How does it account for the variable electrovalency of the elements having configuration of the type ns^2np^{1-4}.

The pair of electron in the valence shell does not take part in bond formation it is called inert pair effect.

19. What is Born-Haber cycle? Explain with an example.

The energy change involved in the formation of an ionic bond from its constituents elements can be represented by an important cycle known as Born-Haber cycle.



Where, $\Delta_{sub}H^{o}$ = Enthalpy of sublimation of sodium metal,

IE = Ionisation energy of sodium,

$\Delta_{disso}H^{o}$ = Enthalpy of dissociation of chlorine molecule,

$\Delta_{eg}H^{o}$ = Electron gain enthalpy of chlorine,

U = Lattice energy of sodium chloride.

20. Discuss the factors which govern the formation of a covalent bond

The factors are :

(i) High value of ionization

(ii) equal electron gain enthalpy

(iii) Equal electronegativities

21. What is variable covalency? Give some examples.

In an excited state, the atom has more probability of sharing its unpaired electron with those of other atoms.

22. What are Sidgwick's views regarding the failure of the octet rule?

According to sidgwick, it is not always necessary for an atom to achieve an octet. He put forward his views in the form of a concept called concept of maximum covalency. In this, the maximum covalency of an atom is governed by its position in periodic table. The maximum covalency of an atom can be less than four as well as it can exceed four.

23. What are Fajan's rules?

The Fajan's rules are :

(i) Smaller size of cation and greater the size of anion, greater is the extent of polarization in an ionic compound.

(ii) Larger the charge on cation and anion, greater is the extent of polarization in an ionic compound.

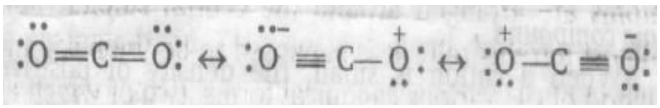
(iii) Higher is the dielectric constant of the medium, lesses is the extent of polarization in an ionic compound.

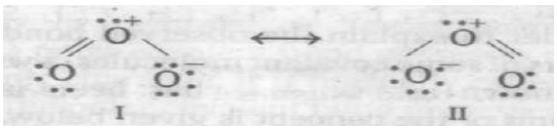
24. Define dipole moment. How is it related to the molecular structure?

Dipole moment is defined as the product of magnitude of the charge present on either of the two atoms and the distance by which the two atoms are separated in the molecule.

Since the dipole moment is a vector quantity, the net dipole moment of a molecule is the resultant of the dipole moments of all the polar bonds present in it.

25. Write the resonating structures of O_3 and CO_2.





26. What is lattice energy and how is it related to the stability of anionic compound?

The amount of energy liberated in condensing the required number of cations and anions to form the lattice of one gram mole of an ionic compound is called the lattice energy of that compound.

The magnitude of lattice energy gives an idea of the inter ionic forces. It depends upon two factors: (i) Smaller the size of ions, greater is the lattice energy, (ii) Higher the charge on the ions, greater is the lattice energy. Lattice energy is regarded as a measure of ease of formation and stability of an ionic compound.

27. Why do covalent compounds exhibit stereoisomerism?

The covalent bonds are rigid and directional. They can orient at specific angles in space. Due to the possibility of different spatial arrangements of covalent bonds in space, a covalent compound may exhibit stereoisomerism.

28. On the basis of VSEPR theory explain why $BeCl_2$ molecule is linear whereas H_2O is angular.

In $BeCl_2$, the central Be atom possesses two bond pairs of electrons. These pairs repel each other to the maximum possible extent and get oriented at an angle of 180°. Therefore, $BeCl_2$ molecule acquires a linear shape.

In H_2O, the two lone pairs of electrons present on the central atom strongly repel the O-H bond pairs. Since lone pair-bond pair repulsion is more than the bond paie-bond pair repulsion, the normal angle of 109° 28’ in a tetrahedral geometry decreases to 104.5° and the tetrahedral geometry gets distorted. The resulting geometry is regarded as bent or angular.

29. What type of forces come into action when two atoms approach each other?

Electron-nucleus attraction, electron-electron repulsion and nucleus-nucleus repulsion.

30. Discuss how the Valence bond theory explains the pyramidal shape of NH_3 molecule.

Hence, the central N atom in NH3

NH_3 Molecules: In ammonia molecules, the central nitrogen atom ($7N = 1s^2,2s^2,2p_x^1, 2p_y^1, 2p_z^1$) has five electrons in the valence shell. Three electrons are mutually shared with the electrons of three hydrogen atoms to form three N-H bonds. Hence, the central N atom in NH3 is surrounding by three bond pair and one lone pair. The geometry expected for the molecules is tetrahedral since lone pair - bond pair repulsion more than bond pair - bond pair repulsion. As a result , the lone pair of electrons will repel another pair strongly. Therefore three N-H bonds of NH3 are forced slightly closer. This leads to decrease in H-N-H bond angles from a normal angle of a tetrahedron (109.5°) to 107°. The

most favorable arrangement is distorted tetrahedral that is pyramidal. In this, nitrogen atom lies at the center and three hydrogen atoms occupying the triangular base and the orbital with a lone pair of electrons from the apex of the pyramid.

31. Explain the difference between a σ and π-bond.

σ - bond		π - bond	
1	It is formed by head on overlapping of atomic orbital.	1	It is formed by the side wise overlapping of atomic orbitals
2	The overlapping of atomic orbitals is maximum.	2	The overlapping of atomic orbitals is much less.
3	The orbital is symmetrical to rotation about the inter-nuclear axis.	3	The orbital is not symmetrical to rotation about the internuclear axis.
4	The resulting covalent bond is strong.	4	The resulting covalent bond is weaker.

32. Draw the shapes of sp^3, sp^2 and sp hybrid orbitals.

33. Out of σ and π-bonds, which bond is stronger and why?

σ bond, due to a greater overlapping of atomic orbitals.

34. Why are the molecules like He_2, H_3 and H_4 not formed?

Two atoms of hydrogen combine to form a molecule. Each hydrogen atom has one electron in its 1s orbital. When the two H atoms come closer to each other their 1s orbitals overlap each other, and both the available electrons are used up in forming a bond between two H-atoms. Since there is no other electron left, the hydrogen molecule (H_2) has no capacity for bonding with more hydrogen atoms. Therefore, only H_2 exists and molecules likeH_3, H_4 etc are not formed.

35. What do you understand by bond length? On what factors does it depend?

The average distance between the centres of the nuclei of the two bonded atoms in a molecule is termed as the bond length.

It depends on two factors:

(i) Size of atoms: Greater the size of the bonded atoms, greater is the bond length.

(ii) Multiplicity of bonds: Bond length decreases with the increase in the multiplicity of bonds. Thus, the bond length of a double bond is smaller than that of a single bond between the same atoms.

36. Carbon possesses only two unpaired electrons in its valence shell. How does it show a covalency equal to four in most of its compounds?

Since, all the four valences of carbon are identical, 2s electron is shifted to one of the vacant p-orbital with the result four unpaired orbitals are present. these undergo hybridization and form four hybrid orbitals. As a result, carbon now has 4 unpaired valence electrons with which it can form four bonds.

37. Why is hybridisation of atomic orbitals necessary for the formation of a molecule? Illustrate your answer by taking the example of CH_4.

CH_4 is basically a combination of 1 carbon and 4 hydrogen atoms. However, to form this compound the central atom carbon which has 4 valence electrons obtain more electrons from 4 hydrogen atoms to complete its octet. When the electrons are shared between carbon and hydrogen there is a formation of a covalent bond or bonds to be more accurate.

In the hybridization of methane, the central atom carbon is sp^3 hybridized. This is because one 2s orbital and three 2p orbitals in the valence shell of carbon combine to form four sp^3 hybrid orbitals which are of equal energy and shape. Further, four H atoms also use these four sp^3 hybrid orbitals of carbon to form C-H sigma bonds which ultimately leads to the formation of the methane molecule.

38. Why is a molecule involving sp^2 hybridisation trigonal and planar?

sp^2 hybrid orbitals are oriented at an angle of 120^o and lie in the same plane.

39. Explain how the Valence bond theory accounts for a carbon-carbon double bond.

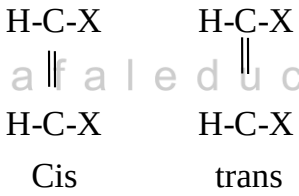
See the formation of C_2H_4 molecule

40. Explain the formation of C_2H_2 molecule.

In C_2H_2, both the carbon atoms are in the sp hybridized state. In the excited state, a 2s and a 2p orbital of each C atom undergo sp hybridization to form two sp hybrid orbitals of equal energy. The other two 2p orbitals of each carbon do not take part in hybridization and remain as pure 2p orbitals even in the hybrid state of the atom. If it is assumed that orbital takes part in hybridization, then each C atom is left with two sp hybrid orbitals lying at 180^o along the X-axis, a pure $2p_y$ orbital lying along Y-axis and a pure $2p_z$ orbital lting along Z-axis.

41. Explain why the compounds of the type $C_2H_2X_2$ exhibit cis-trans isomerism.

The compounds of the type C2H2X2 possess a C=C double bond. Atoms cannot rotate around a double bond. Therefore, following two orientations of atoms in space are possible.



The isomer in which similar atoms are on the same side of double bond is called a cis isomer while that in which similar atoms are on the opposite sides is called a trans isomer and the compound is said to show cis-trans isomerism.

42. Why does a covalent bond develop a partial ionic character when the electronegativities of the combining atoms are different?

When a covalent bond is formed between two atoms of different electronegativities, the more electronegative atom tries to pull the shared pair of electrons to a greater extent towards its own side. As a result, the shared pair gets shifted towards the more electronegative atom. This distorts the electron charge cloud. Consequently, the more electronegative atom acquires a partial negative charge and the less electronegative atom a partial positive charge. Thus, the bond develops a partial ionic character.

43. How do the metals conduct heat and electricity?

The electrons in metal are delocalized electrons and are free moving electrons so when they gain energy (heat) they vibrate more quickly and can move around, this means that they can pass on the energy more quickly.

Metals conduct electricity by allowing free electrons to move between the atoms. These electrons are not associated with a single atom or covalent bond. Since like charges repel each other, the movement of one free electron within the lattice dislodges those in the next atom, and the process repeats – moving in the direction of the current, toward the positively charged end.

44. Explain why (i) metals are malleable and ductile; (ii) sodium can be cut with a knife; (iii) H_2O is a liquid while H_2S is a gas; (iv) o-nitrophenol possesses low boiling point inspite of the presence of hydrogen bonding in it.

(iv) The hydrogen bonding present in o-nitrophenol is intramolecular. Intramolecular hydrogen bonding does not associate molecules. This is why o-nitrophenol has a low boiling point.

45. What do you understand by overlap integral and what does it signify?

The strength of covalent bond thus formed depends upon the extent of overlapping which is given by an integral S, known as overlap integral.

46. State the salient features of molecular orbital theory.

(1) When two atoms approach each other, their atomic orhitals lose, their identity and mutually overlap to form new orbitals called molecular orbitals.

(2) Molecular orbitals are associated with the molecule as a whole and are quantised.

(3) The molecular orbitals are polycentric. They surround the nuclei of the combining atoms and the electrons are considered moving over the whole nuclear system instead of moving around a particular nucleus.

(4) (iv) Molecular orbitals are formed only by those atomic orbitals which are of comparable energies and possesse proper orientation.

(5) The number of molecular orbitals formed is the same as the number of combining atomic orbitals.

(6) A molecular orbital can accommodate a maximum of two electrons.

(7) The molecular orbitals are filled within the framework of the same rules as applied for the filling_atomic orbitals i.e., Pauli's exclusion, principle, Hund's rule and aufbau principle.

(8) The shape of a molecular orbital depends upon the shapes of combining atomic orbitals

47. What are the main points of difference between atomic and molecular orbitals?

	Atomic orbitals		Molecular orbitals
1	In an atomic orbital, the electron cloud is associated with the nucleus of a single atom. Thus an atomic orbital is monocentric.	1	In a molecular orbital, the electron cloud is associated with the molecule as a whole and is spread over the whole nuclear

			system of combining atoms. A molecular orbit is thus polycentric.
2	They are pure orbitals and obtain by solving Schrodinger wave equation for the given atomic system.	2	They are usually obtain by the combination of atomic orbitaks of the combining atoms.
3	They possess higher energy and are less stable.	3	The bonding molecular orbits possess lesser energy and are more stable.

48. What do you understand by linear combination of atomic orbitals?

The process of approximating the correct molecular orbitals by combining the atomic orbitals of the combining atoms is called linear combination of atomic orbitals.

49. Explain why a bonding molecular orbital is of low energy while an antibonding molecular orbital of high energy.

A bonding molecular orbital is formed when the electron waves of the combining atoms are in phase i.e., both have positive (+) amplitude. In this molecular orbital, the electron density is centred between the nuclei of the combining atoms. It shields the two nuclei from mutual repulsion and holds them at a definite distance which is equal to the bond length. Due to increased attraction between the two atoms^ the energy of the system decreases. This is why a bonding molecular orbital is a low energy orbital.

An antibonding molecular orbitals formed when the electron waves of the combining atoms are not in phase i.e., one possesses positive (+) amplitude while the other possess a negative (-) amplitude. In this case, the wave functions of the component atoms cancel each other and form a node between the nuclei. In such an orbital, electrons are in those regions of space where they are not under the attraction of both the nuclei. The probability of finding the electron between the nuclei is negligible, thus the two nuclei repel each other and make the molecule unstable. Each electron in an antibonding molecular orbital contributes to the repulsion and increases the energy of the system. Thus, an antibonding molecular orbital is a repulsive orbital of higher energy.

50. What are the main points of difference between bonding and antibonding molecular orbitals?

Bonding molecular orbitals		Antibonding molecular orbitals	
1	A bonding molecular orbital is formed when the electron waves of combining atoms are in phase, i.e.,the lobes of atomic orbitals have same sign	1	An antibonding molecular orbital is formed when the electron waves of the combining atoms are not in phase, i.e., the lobes of atomic orbitals have opposite sign.
2	The wave function for a bonding molecular orbital may be approximated by summing up the wave functions of the combining atoms, i.e., $\Psi_b = \Psi_A + \Psi_B$	2	The wave function for an antibonding molecular orbital is obtained by subtracting the wave functions of the combining atoms, i.e., $\Psi_a = \Psi_A - \Psi_B$

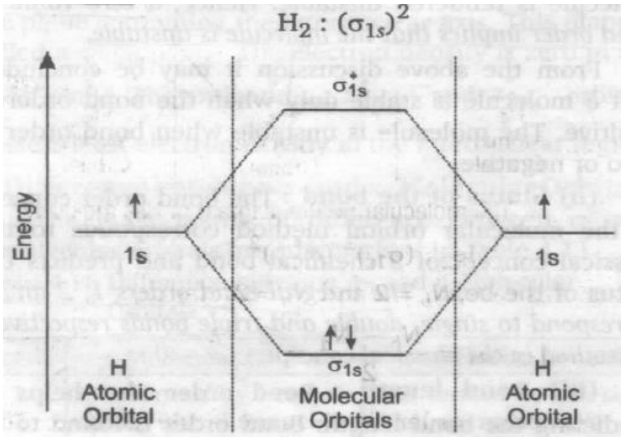
3	The electron density is centred between the nuclei of the combining atoms.	3	The probability of finding the electron between the nuclei of the combining atoms is negligible.
4	The energy of a bonding molecular orbital is less than that of the atomic orbitals of combining atoms	4	The energy of an antibonding molecular orbital is greater than that of the atomic orbitals of combiningatoms
5	Electrons present in bonding molecular orbitals lead to attraction between the atoms and stabilize the molecule	5	Electrons present in antibonding molecular orbitals lead to repulsion between the atoms and destabilize the molecule

51. What are the main points of difference between σ and π orbitals?

	σ molecular orbitals		**π molecular orbitals**
1	It is formed by head on (along inter-nuclear axis) overlapping of atomic orbitals.	1	It is formed by the side wise (perpendicular to the inter-nuclear axis) overlapping of atomic orbitals.
2	The overlapping of atomic orbitals is maximum.	2	The overlapping of atomic orbitals is much less.
3	The orbital is symmetrical to rotation about the internuclear axis.	3	The orbital is not symmetrical to rotation about the internuclear axis.
4	The resulting covalent bond is strong.	4	The resulting covalent bond is weaker.

52. Give the molecular orbital description of hydrogen molecule and deduce the bond order.

Hydrogen molecule (H_2) is formed by the combination of two hydrogen atoms. Hydrogen atom ($1s^1$) contains only one electron in ls-atomic orbital. H_2 molecule will thus possess two electrons. At a certain internuclear distance, the ls-atomic orbitals of the two combining H-atoms overlap to form σ_{1s} and σ^*_{1s} molecular orbitals. According to aufbau principle, the two electrons of the combining hydrogen atoms should be placed in the low energy σ_{1s} orbital. The high energy σ^*_{1s} orbital remains vacant. The molecular orbital electronic configuration of H2 molecule is therefore $(\sigma_{1s})^2$.



$$\text{Bond order} = \frac{N_b - N_a}{2} = \frac{2-0}{2} = 1.$$

53. Distinguish two aspects of bonding and antibonding molecular orbitals.

(1) Bonding orbitals place most of the electron density between the nuclei of the bonded atoms. Antibonding orbitals place most of the electron density outside the nuclei.

(2) Electrons in bonding orbitals stabilize the molecule because they are between the nuclei. They also have lower energies because they are closer to the nuclei. Antibonding orbitals place less electron density between the nuclei. The nuclear repulsions are greater, so the energy of the molecule increases. Antibonding orbitals are at higher energy levels than bonding orbitals.

(3) The main difference between bonding and antibonding molecular orbitals is that bonding molecular orbitals represent the shape of a molecule whereas antibonding molecular orbitals do not contribute to the determination of the shape of a molecule.

54. Describe molecular orbital. How is it different from an atomic orbital?

Molecular orbital theory was proposed by Mulliken, Huckel and Hund. According to this theory, when two atoms approach each other, their atomic orbitals lose their identity and mutually overlap to form new orbitals called molecular orbitals.

55. Why does He_2 not exist?

The bond order for He_2 is zero. Hence, the molecule cannot exist.

56. What do you understand by bond order and what does it signify?

The amount of energy required to break one mole of bonds of the same kind to separate the bonded atoms in the gaseous state is called the bond energy.

The magnitude of bond energy is a measure of the strength of the bond.

57. Why is bond order in H_2^- less than that in H_2?

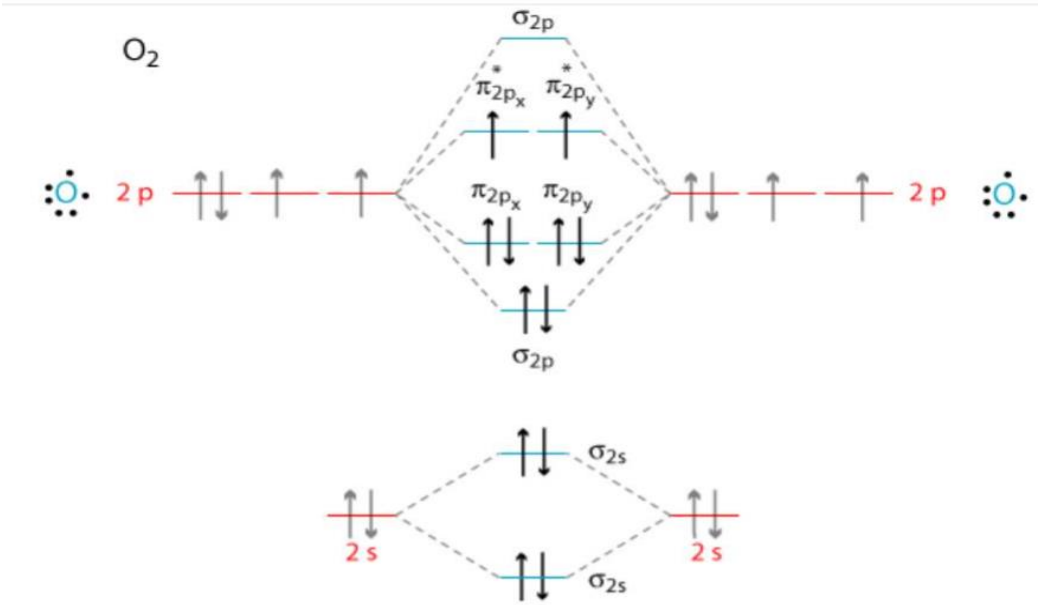
Hydrogen molecule (H_2) is formed by the combination of two hydrogen atoms. Hydrogen atom ($1s^1$) contains only one electron in ls-atomic orbital so, its molecular orbital electronic configuration is therefore $(\sigma_{1s})^2$. Therefore its bond order is

$$\text{Bond order} = \frac{N_b - N_a}{2} = \frac{2-0}{2} = 1.$$

The hydrogen molecular anion (H_2^-) is formed by the combination of a hydrogen atom (containing one electron in l s-orbital) and a hydride ion H^- (containing two electrons in l s orbital). Thus in all, H_2^- ion contains 3 electrons. The two electrons occupy σ_{1s}-orbital and the remaining third electron goes to σ^*_{1s} orbital. Thus; the molecular orbital electronic configuration of H_2^- ion is $(\sigma_{1s})^2(\sigma^*_{1s})^1$. Therefore, its bond order is

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

58. Explain on the basis of molecular orbital diagram why O_2 should be paramagnetic.



Electron Configuration: $(\sigma_{2s})^2\ (\sigma_{2s}^*)^2\ (\sigma_{2p})^2\ (\pi_{2p})^4\ (\pi_{2p}^*)^2$

Bond Order $= \frac{1}{2}(2 - 2 + 2 + 4 - 2) = 2$ Double Bond

From the molecular orbital diagram of O_2 shown in Fig., it is clear that the aufbau order of filling of molecular orbitals leaves two unpaired electrons, one each in π^*_{2Px} and π^*_{2py} molecular orbitals. Thus, a O_2 molecule possesses two unpaired electrons even in the ground state. The unpaired electrons impart paramagnetic character to oxygen molecule. Thus, O_2 molecule should be paramagnetic in nature.

59. Using molecular orbital diagram, arrange the following molecular species in the increasing order of their stabilities: H_2, H_2^+ and H_2^-.

$H^{2-} < H^{2+} < H^2$

60. Which of the following species are paramagnetic? H_2, H_2^+ and H_2^-.

H^{2+} and H^{2-}

61. With the help of molecular orbital approach show the Ne_2 cannot exist as a stable species.

The molecular orbital electronic configuration of Ne_2 molecule can be written as follows:

Ne_2 : KK $(\sigma_{2s})^2\ (\sigma^*_{2s})^2(\sigma_{2pz})^2\ (\pi_{2px})^2\ (\pi_{2py})^2\ (\pi^*_{2px})^2\ (\pi^*_{2py})^2\ (\sigma^*_{2pz})^2$

In this case, $N_b = 8$ and $N_a = 8$. Hence

$$\text{Bond order} = \frac{N_b - N_a}{2} = \frac{8 - 8}{2} = 0$$

The zero value of bond order signifies that no bond exists between two neon atoms in Ne_2 molecule. This implies that Ne_2 molecule cannot exist.

62. Arrange the following molecular species in increasing order of stability (giving bond orders) : O_2, O_2^+, O_2^-, O_2^{2-}

$O_2^{2-} < O_2^- < O_2 < O_2^+$ B.O. 1, 3/2, 2, 5/2

63. What are the main points of difference between valence bond and molecular orbital theories?

64. Depict molecular orbital diagrams of N_2^+ and He_2^+ and predict which one of the two species will be more stable.

65. Define hybridization.

Hybridization may be defined as the phenomenon of intermixing of atomic orbitals of comparable energies to form a set of same number of new orbitals of equal energy and identical in all hybrid orbitals.

66. Give reason for the following: Bond order in N_2 is 3 whereas it is 2.5 in NO.

Review Exercise – 1

1. **Why do atoms combine together?**

   Atoms of elements other than noble gases or inert gases are usually less stable. Consequently, the atoms of such elements show a great tendency to combine with other atoms of the same or different elements to form compounds and attain stability. In other words, atoms are looking to attain a stable electronic configuration octet structure. The target is of the nearest noble gas in the periodic table.

2. Give the Lewis structures and the formulae of the ionic compound formed by the combination of the following pairs of elements:

   (1) Na, I

   (2) Ca, O

   (3) K, S

   (4) Mg, N.

3. **Discuss the feasibility of the formation of an ionic bond if**

   (1) IE of electropositive atom is high and EA of electronegative atom is low;

   If the ionization energy of electropositive atom is high that means it does not lose an electron easily and in the second electronegative atom the electron affinity is low which means it has less tendency to gain an electron. So both the atoms are not favoring the formation of an ionic bond.

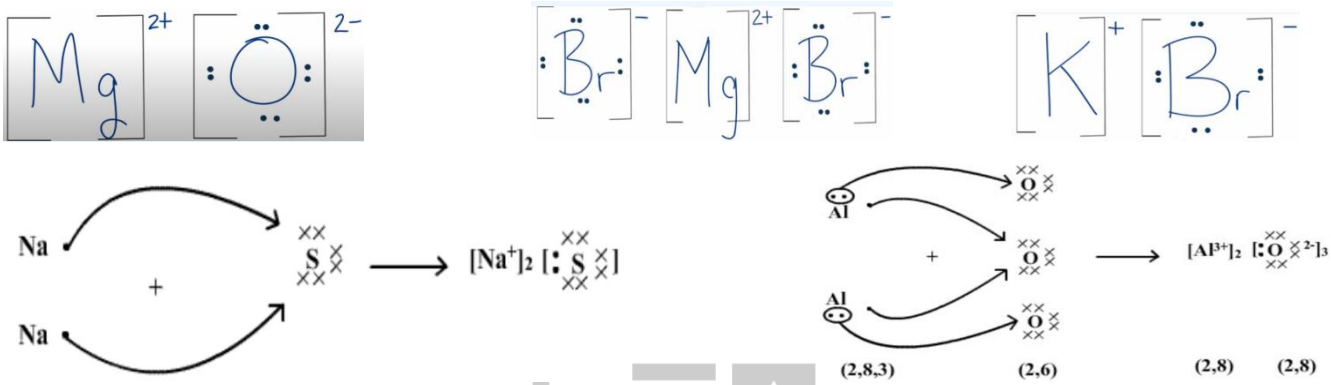
   (2) IE of electropositive atom is low and EA of electronegative atom is high;

   If the ionization energy of electropositive atom is low that means it can readily lose an electron and similarly the high electron affinity of electronegative atom favor the atom to gain an electron easily. So in this case the feasibility of formation of an ionic bond is very high.

   (3) both the atoms are of equal electronegativities.

If the electronegativity of both the atoms is same then the electronegativity difference between them is zero and the ability of both the atom to attract or lose the electron is same and hence no transfer of electron takes place and there is no chance of formation of ionic bond.

4. **Write the electron dot structures of the following compounds: MgO, MgBr2, KBr, Na2S and Al2O3**



5. **Explain why**

(1) ionic compounds possess very high melting and boiling points?

The positive and negative ions formed during ionic bonding are held together by enormously strong forces of attraction between the oppositely charged ions. These ionic bonds between the charged particles result in a giant structure of ions. Because the ions are held together tightly in this giant structure it takes a lot of energy to break all the bonds. As a result, ionic compounds have high melting and boiling points.

(2) ionic compounds are soluble in water but insoluble in organic solvents?

The water molecules have high dielectric constant thus, water molecules easily break the ionic bonds between the ions. The ions drift in water in all possible directions and hence, ionic compounds dissolve in water, while organic solvents are non-polar in nature and hence, cannot break the ionic bonds. Thus, the ionic compounds do not dissolve in them.

(3) ionic compounds are hard and brittle?

The ionic solids are hard and brittle because the ions in ionic solids are held in a lattice due to the electrostatic forces of attraction in cation and anions as well as the repulsion with the like charges. Thus, the Ionic solids are hard due to the presence of strong electrostatic forces of attraction. The brittleness in ionic crystals is due to the non-directional nature of the ionic bonds in them.

(4) An ionic bond cannot be formed between the atoms of the same element?

In ionic bonding, atoms transfer electrons to each other. Ionic bonds require at least one electron donor and one electron acceptor. In contrast, atoms with the same electronegativity share electrons in covalent bonds, because neither atom preferentially attracts or repels the shared electrons. For example: carbon does not form ionic bonds because it has 4 valence electrons, half of an octet. To form ionic bonds, Carbon molecules must either gain or lose 4 electrons. Thus, An ionic bond cannot be formed between the atoms of the same element.

(5) lonic reactions are very fast.

6. What is octet rule? Illustrate it with some examples.