Examples:

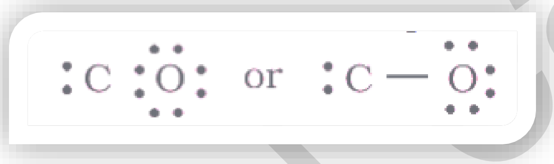
4.1 Write the Lewis dot structure of CO molecule.

Answer:

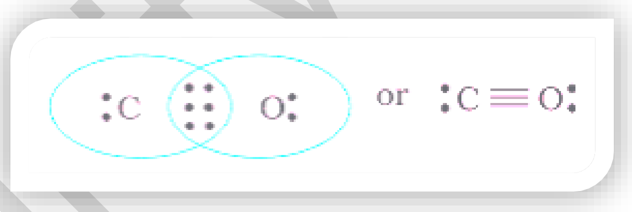
Step 1: Count how many valence electrons each carbon and oxygen atom have. Carbon and oxygen atoms' outer (valence) shell configurations are $2s^2\ 2p^2$ and $2s^2\ 2p^4$, respectively. $4 + 6 = 10$ valence electrons are accessible.

Step 2: CO is written as $C\ O$ in its skeletal structure.

Step 3: Complete the octet on O by drawing a single bond (one shared electron pair) between C and O; the remaining two electrons are the lone pair on C.



Because this does not complete the octet on carbon, we must use multiple bonding (in this case a triple bond) between the C and O atoms. For both atoms, this meets the octet rule prerequisite.



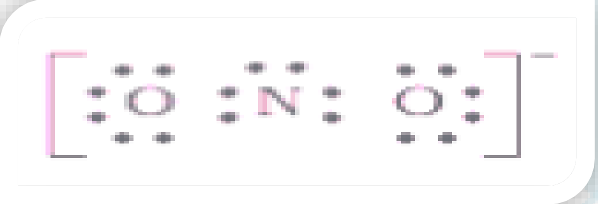
4.2 Write the Lewis structure of the nitrite ion NO_2^- .

Answer:

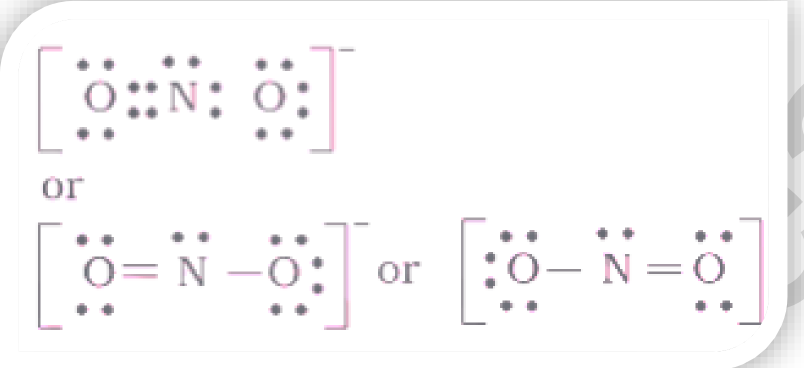
Step 1: Count the total number of valence electrons in the nitrogen, oxygen, and one more negative charge atoms (equal to one electron). $5 + (2\ 6) + 1 = 18$ electrons $N\left(2s^2\ 2p^3\right)$, $O\ \left(2s^2\ 2p^4\right)$

Step 2: NO_2^- has the following skeleton structure: $O\ N\ O$

Step 3: To complete the octets on oxygen atoms, draw a single bond (one shared electron pair) between the nitrogen and each of the oxygen atoms. However, if the remaining two electrons form a lone pair on nitrogen, this does not complete the octet.



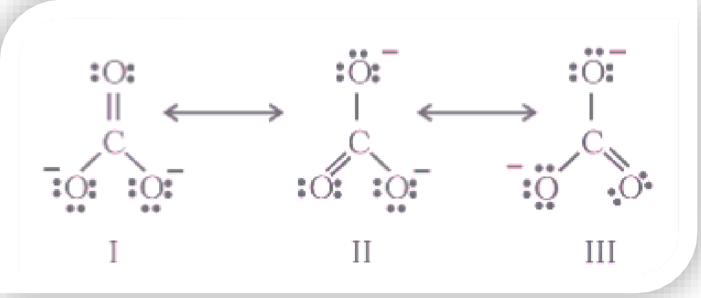
As a result, multiple bonding between nitrogen and one of the oxygen atoms is required (in this case a double bond). The Lewis dot structures that result are as follows.



4.3 Explain the structure of CO_3^{2-} ion in terms of resonance.

Answer:

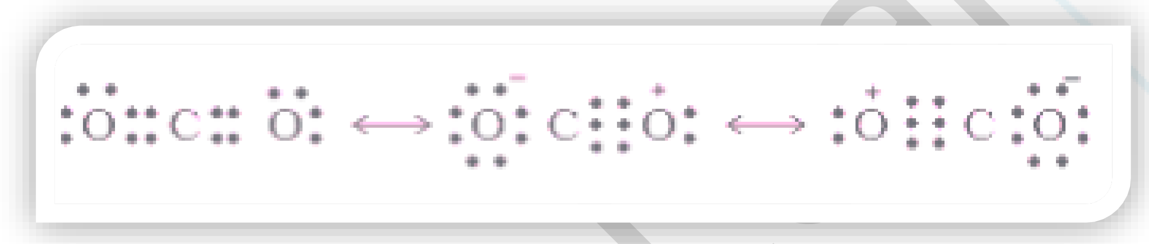
Because it represents unequal bonds, the single Lewis structure based on the presence of two single bonds and one double bond between carbon and oxygen atoms is insufficient to adequately represent the molecule. All carbon to oxygen bonds in CO_3^{2-} is comparable, according to the experimental data. As a result, the carbonate ion is best represented as a resonance hybrid of the three classical forms indicated below.



4.4 Explain the structure of $\mathrm{CO_2}$ molecule.

Answer:

The carbon to oxygen bond length in CO_2 has been determined experimentally to be $115\ pm$. The lengths of carbon to oxygen double bonds $(C=O)$ and carbon to oxygen triple bonds $(C=O)$ are 121 and $110\ pm$, respectively. CO_2 $(115\ pm)$ has carbon-oxygen bond lengths that are halfway between $C=O$ and CO. CO_2's structure is a hybrid of canonical and resonance forms I, II, and III. Obviously, a single Lewis structure cannot depict this position, as a result, various Lewis structures must be written, and it is preferable to think of CO_2's structure as a mix of the canonical or resonance forms I, II, and III.



Exercise:

4.1 Explain the formation of a chemical bond.

Answer:

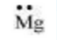
A chemical bond is an attractive force that holds the elements of a chemical species together (atoms, ions, etc.).

For the creation of chemical bonds, various theories have been proposed, including the electronic theory, valence shell electron pair repulsion theory, valence bond theory, and molecular orbital theory.

The tendency of a system to achieve stability is related to the development of chemical bonds. Noble gases' inertness was discovered to be due to their entirely filled outermost orbitals. As a result, it was hypothesized that elements with incomplete outermost shells are unstable (reactive). To achieve the stable configuration of the closest noble gases, atoms interact with one another and complete their respective octets or duplets. This can happen when electrons are shared or when one or more electrons are transferred from one atom to another. A covalent bond is a chemical link established as a result of the sharing of electrons between atoms. An ionic link is established when electrons are transferred from one atom to another.

4.2 Write Lewis dot symbols for atoms of the following elements: Mg, Na, B, O, N, Br.

Answer:

Mg : There are two valence electrons in Mg atom. Hence, the Lewis dot symbol for Mg is: 

Na : There is only one valence electron in a sodium atom. As a result, the Lewis dot structure is as follows: $Na^{\bullet}$

B : Boron atoms have three valence electrons. As a result, the Lewis dot structure is as follows: $\bullet\underset{\bullet}{B}\bullet$

O : In an atom of oxygen, there are six valence electrons. As a result, the Lewis dot structure is as follows: 

N : In a nitrogen atom, there are five valence electrons. As a result, the Lewis dot structure is as follows: 

Br : Bromine contains seven valence electrons. As a result, the Lewis dot structure is as follows:

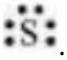
4.3 Write Lewis symbols for the following atoms and ions:

S and S^{2-} ; Al and Al^{3+} ; H and H^{-}

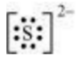
Answer:

(i) S and S^{2-}

Sulphur has a total of six valence electrons. Sulphur (S) has a Lewis dot symbol.

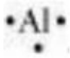


In addition to the six valence electrons, the dinegative charge implies that there will be two additional electrons. As a result, S^{2-} Lewis –'s dot sign is



(ii) Al and Al^{3+}

Aluminium has a total of three valence electrons. Aluminium (Al) has a Lewis dot symbol.



A species' tripositive charge indicates that its three electrons have been contributed.

As a result, the Lewis dot sign $[Al]^{3+}$.

(iii) H and H–

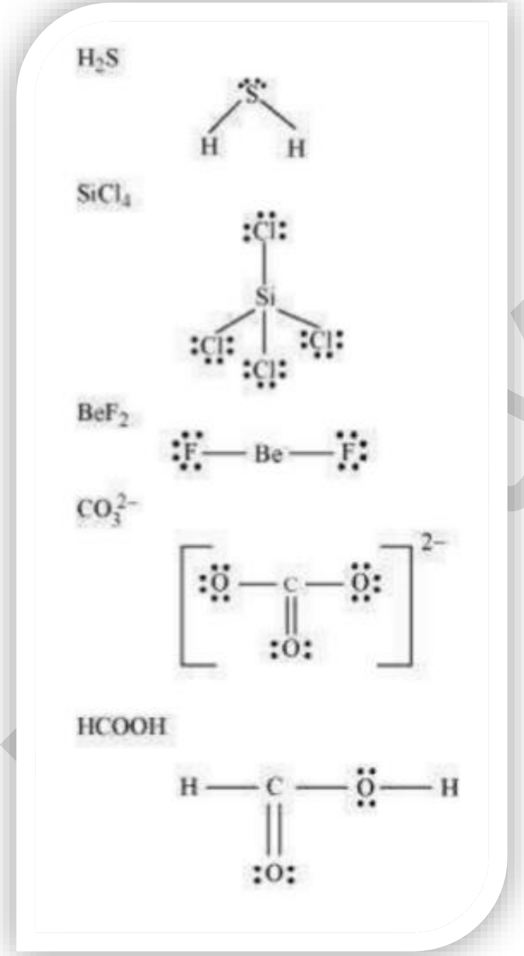
Hydrogen has a valence electron count of one. Hydrogen (H) is represented by the Lewis dot symbol. $H^{\bullet}$.

In addition to the one valence electron, the uni-negative charge implies that there will be one extra electron. As a result, the Lewis dot sign $\left[\overset{\bullet\bullet}{H}\right]^{-}$.

4.4 Draw the Lewis structures for the following molecules and ions:

H_2S, $SiCl_4$, BeF_2, CO_3^{2-}, HCOOH

Answer:



4.5 Define octet rule. Write its significance and limitations.

Answer:

Kossel and Lewis created the octet rule, or electrical theory of chemical bonding.

According to this rule, atoms can interact by transferring valence electrons between them or by sharing their valence electrons in order to achieve the nearest noble gas configuration by having an octet in their valence shell.

The octet rule successfully defined how chemical bonds develop depending on the element's nature.

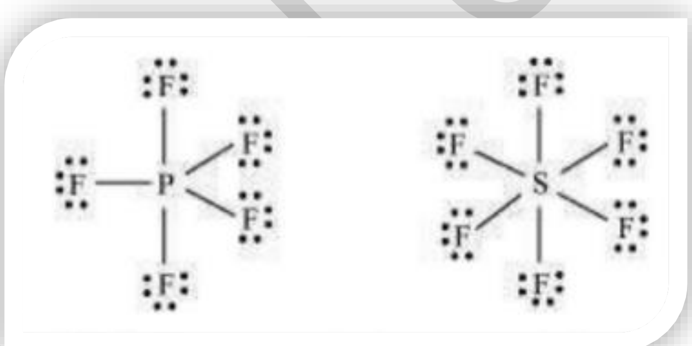
The octet theory's drawbacks include:

The octet rule has the following limitations:

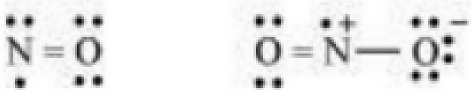
(a) The rule was unable to predict molecular shape and relative stability.

(b) It is based on noble gases' inert properties. Some noble gases, such as xenon and krypton, do, nevertheless, form compounds such as XeF_2, KrF_2, and others.

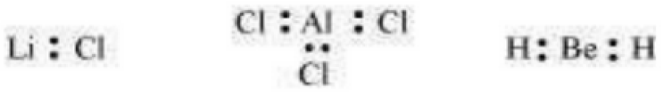
(c) The octet rule does not apply to elements in and beyond the periodic table's third period. More than eight valence electrons surround the core atom in the elements found in these eras. For instance, PF_5, SF_6, and so on.



(d) For all atoms in a molecule with an odd number of electrons, the octet rule is violated. The octet rule is not satisfied by NO and NO_2. central atom.



(e) This rule does not apply to compounds with less than eight electrons surrounding the core atom. $LiCl$, BeH_2, $AlCl_3$, and other compounds defy the octet rule.



4.6 Write the favorable factors for the formation of ionic bond.

Answer:

The transfer of one or more electrons from one atom to other forms an ionic connection. As a result, the ease with which neutral atoms can lose or receive electrons determines the development of ionic bonds. Bond formation is also influenced by the compound's lattice energy.

As a result, the following are favorable circumstances for the development of ionic bonds:

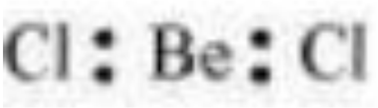
(i) Metal atoms with a low ionisation enthalpy.
(ii) A non-metal atom with a high electron gain enthalpy $\left(\Delta eg\ H\right)$.
(iii) The chemical created has a high lattice energy.

4.7 Discuss the shape of the following molecules using the VSEPR model:

$BeCl_2$, BCl_3, $SiCl_4$, AsF_5, H_2S, PH_3

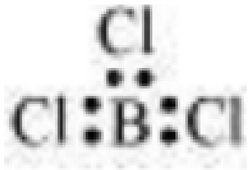
Answer:

$BeCl_2$:

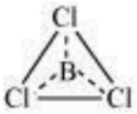


On the central atom, there are two bond pairs and no lone pairs. $BeCl_2$ belongs to the AB_2 type. As a result, it has a linear form.

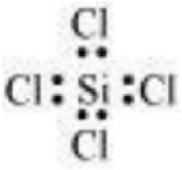
BCl_3:



There are three bond pairs and no lone pairs on the centre atom. As a result, it belongs to the AB_3 type. As a result, it's trigonal planar.

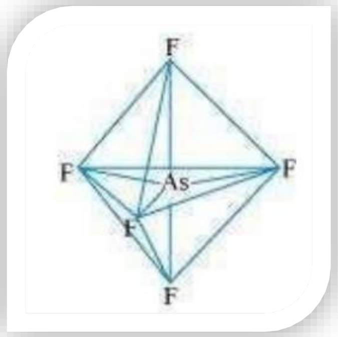


$SiCl_4$:



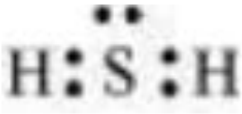
On the central atom, there are four bond pairs and no lone pairs. As a result, $SiCl_4$ is a tetrahedral AB_4 type molecule with a tetrahedral form.

AsF_5 :



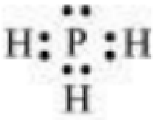
There are five bond pairs and no lone pairs on the centre atom. As a result, AsF_5 belongs to the AB_5 type. As a result, the form is trigonal bipyramidal.

H_2S:



There is one lone pair on the centre atom and two bond pairs. As a result, H_2S is of type AB_2E. Bent is the shape.

PH_3:

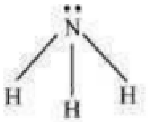


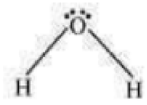
There is one lone pair on the centre atom and three bond pairs. As a result, PH_3 belongs to the AB_3E family. As a result, the form is trigonal bipyramidal.

4.8 Although geometries of NH_3 and H_2O molecules are distorted tetrahedral, bond angle in water is less than that of ammonia. Discuss.

Answer:

The molecular geometry of NH_3 and H_2O may be proven as:





The significant atom (N) in NH_3 has one lone pair and there are 3 bond pairs. In H_2O, there are lone pairs and bond pairs.

The lone pairs gift withinside the oxygen atom of H_2O molecule repels the 2 bond pairs. This repulsion is more potent than the repulsion among the lone pair and the 3 bond pairs at the nitrogen atom.

Since the repulsions at the bond pairs in H_2O molecule are extra than that during NH_3, the bond perspective in water is much less than that of ammonia.

4.9 How do you express the bond strength in terms of bond order?

Answer:

Bond energy represents the volume of bonding among atoms forming a molecule. The large the bond energy, the more potent is the bond and the extra is the bond order.

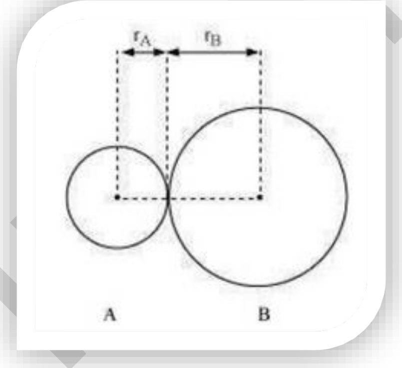
4.10 Define the bond length.

Answer:

Bond duration is described because the equilibrium distance among the nuclei of bonded atoms in a molecule.

Bond lengths are expressed in phrases of Angstrom $\left(10^{-10}\ m\right)$ or picometer $(10^{-12}\ m)$ and are measured with the aid of using spectroscopic X-ray diffractions and electron-diffraction techniques.

In an ionic compound, the bond period is the sum of the ionic radii of the constituting atoms $\left(d = r_+ + r_-\right)$. In a covalent compound, it's miles the sum in their covalent radii $\left(d = r_A + r_B\right)$.



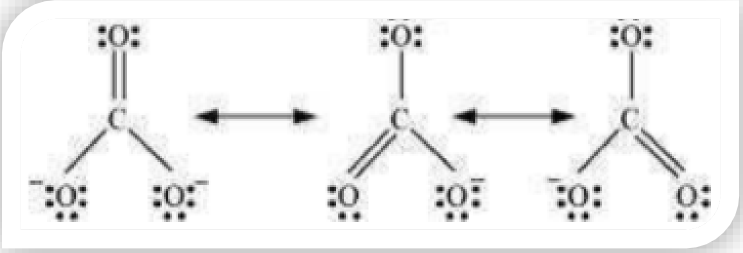
4.11 Explain the important aspects of resonance with reference to the CO_3^{2-} ion.

Answer:

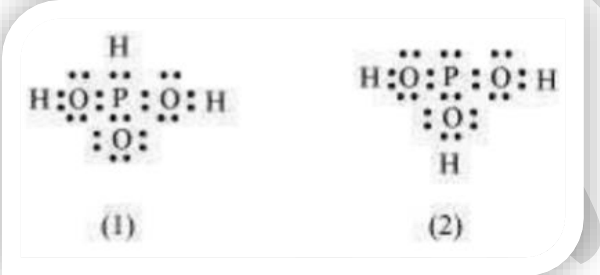
According to experimental findings, all carbon to oxygen bonds in CO_3^{2-} are equivalent.

Hence, it's far insufficient to represent CO_3^{2-} ion with the aid of using a unmarried Lewis shape having unmarried bonds and one double bond.

Therefore, carbonate ion is defined as a resonance hybrid of the subsequent structures:



4.12 H_3PO_3 can be represented by structures 1 and 2 shown below. Can these two structures be taken as the canonical forms of the resonance hybrid representing H_3PO_3? If not, give reasons for the same.



Answer:

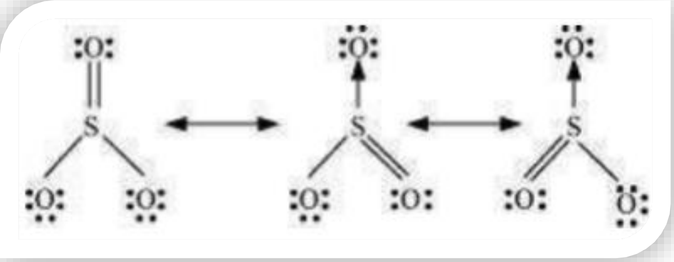
The given systems cannot be taken because the canonical types of the resonance hybrid of H_3PO_3 due to the fact the positions of the atoms have changed.

4.13 Write the resonance structures for SO_3, NO_2 and NO_3^-.

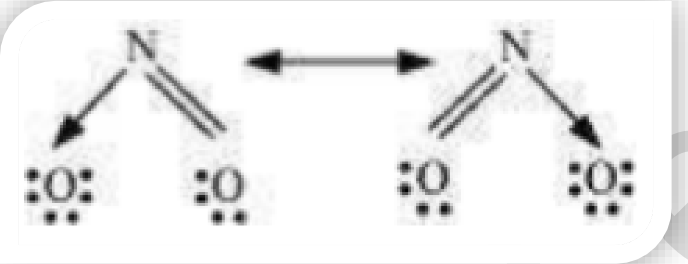
Answer:

The resonance systems are:

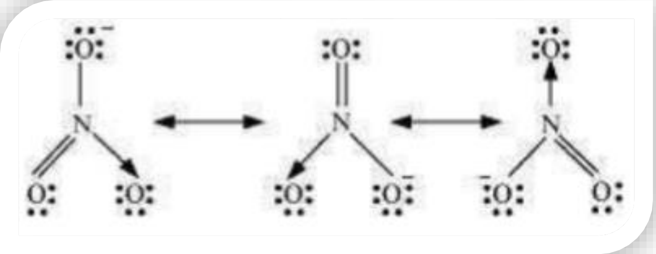
(a) SO_3



(b) **NO_2**



(c) **NO_3^-**



4.14 Use Lewis symbols to show electron transfer between the following atoms to form cations and anions: (a) K and S (b) Ca and O (c) Al and N.

Answer:

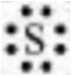
K and **S**:

The digital configurations of K and S are as follows:

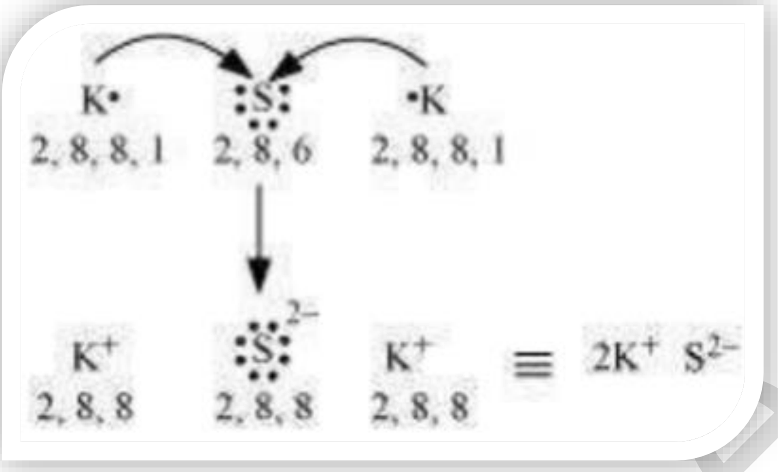
$K:\ 2,\ 8,\ 8,\ 1$

$S:\ 2,\ 8,\ 6$

K •



Sulphur (S) calls for 2 extra electrons to finish its octet. Potassium (K) calls for one electron extra than the closest noble fueloline i.e., Argon. Hence, the electron switch may be proven as:



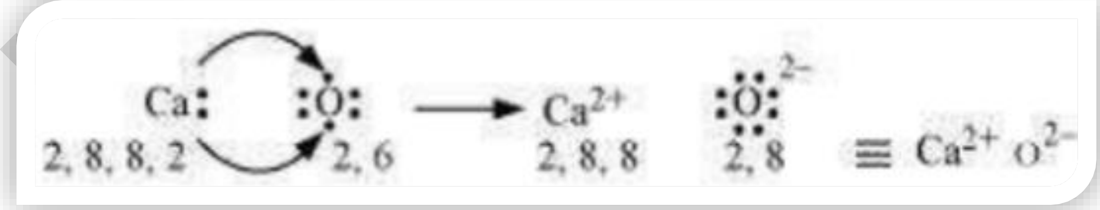
(b) **Ca** and **O**:

The digital configurations of **Ca** and **O** are as follows:

Ca: 2, 8, 8, 2

O: 2, 6

Oxygen calls for electrons greater to finish its octet, while calcium has electrons greater than the closest noble fueloline i.e., Argon. Hence, the electron switch takes area as:



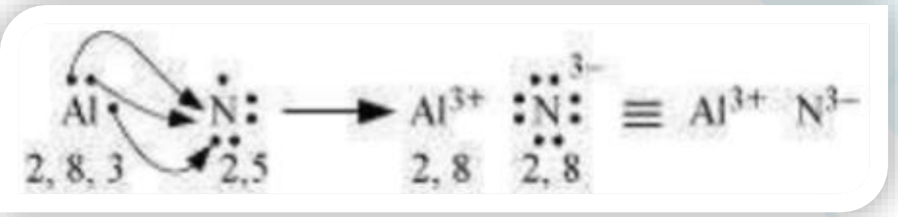
(c) Al and N:

The digital configurations of Al and N are as follows:

Al: 2, 8, 3

N: 2, 5

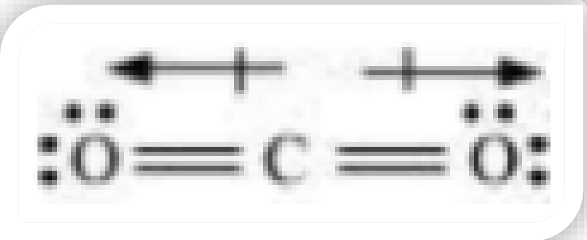
Nitrogen is 3 electrons brief of the closest noble gas (Neon), while aluminium has 3 electrons greater than Neon. Hence, the electron transference may be proven as:



4.15 Although both CO_2 and H_2O are triatomic molecules, the shape of H_2O molecule is bent while that of CO_2 is linear. Explain this on the basis of dipole moment.

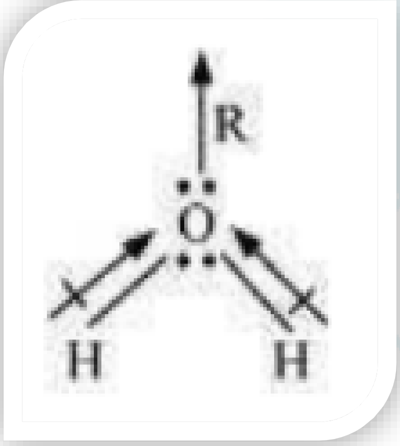
Answer:

According to experimental results, the dipole second of carbon dioxide is zero. This is viable handiest if the molecule is linear in order that the dipole moments of $C-O$ bonds are identical and contrary to nullify every other.



Resultant $\mu = 0\,D$

H_2O, on the alternative hand, has a dipole second fee of aleven though it's far a triatomic molecule as CO_2). The fee of the dipole second indicates that the shape of H_2O molecule is bent in which the dipole second of O–H bonds are unequal.



4.16 Write the significance/applications of dipole moment.

Answer:

In heteronuclear molecules, polarization arises because of a distinction withinside the electronegativities of the parts of atoms. As a result, one cease of the molecule acquires a high-quality price at the same time as the alternative cease turns into negative. Hence, a molecule is stated to own a dipole.

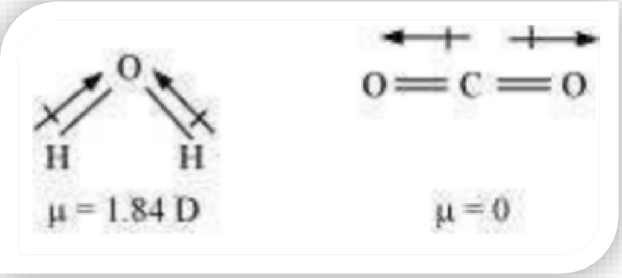
The made of the value of the rate and the space among the centres of superb-poor costs is referred to as the dipole moment (μ) of the molecule. It is a vector amount and is represented through an arrow with its tail on the superb centre and head pointing closer to a poor centre.

Dipole moment (μ) = charge $(Q) \times$ distance of separation (r).

The SI unit of a dipole second is 'esu'.

$$1\ esu = 3.335 \times 10^{-30}\ cm$$

Dipole second is the degree of the polarity of a bond. It is used to distinguish among polar and non-polar bonds in view that all non-polar molecules $(e.g.\ H_2,\ O_2)$ have 0 dipole moments. It is likewise useful in calculating the share ionic individual of a molecule.



4.17 Define electronegativity. How does it differ from electron gain enthalpy?

Answer:

Electronegativity is the capacity of an atom in a chemical compound to draw a bond pair of electrons toward itself.

Electronegativity of any given detail isn't regular. It varies in line with the detail to which it's far bound. It isn't a measurable quantity. It is best a relative number.

On the alternative hand, electron benefit enthalpy is the enthalpy alternate that takes vicinity whilst an electron is introduced to a impartial gaseous atom to shape an anion. It may be poor or nice relying upon whether or not the electron is introduced or removed. An detail has a regular price of the electron benefit enthalpy that may be measured experimentally.

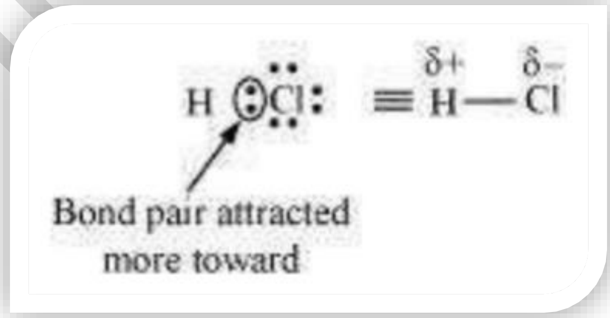
4.18 Explain with the help of suitable example polar covalent bond.

Answer:

When numerous atoms having distinct electronegativities integrate to shape a covalent bond, the bond pair of electrons isn't shared equally. The bond pair shifts closer to the nucleus of the atom having more electronegativity. As a result, electron distribution gets distorted, and the electron cloud is displaced towards the electronegative atom.

As a result, the electronegative atom will become barely negatively charged at the same time as the alternative atom will become barely undoubtedly charged. Thus, contrary poles are evolved withinside the molecule and this sort of a bond is referred to as a polar covalent bond.

HCl, for example, contains a polar covalent bond. Chlorine atom is more electronegative than hydrogen atom. As a result, the bond pair is oriented towards chlorine, giving it a partial negative charge.



4.19 Arrange the bonds in order of increasing ionic character in the molecules: LiF , K_2O , N_2 , SO_2 and ClF_3 .

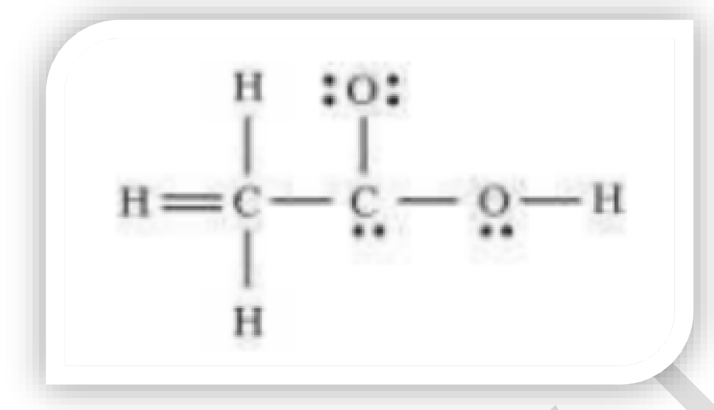
Answer:

The ionic man or woman in a molecule relies upon the electronegativity distinction among the constituting atoms. The more the distinction, the more could be the ionic man or woman of the molecule.

On this basis, the order of growing ionic man or woman withinside the given molecules are

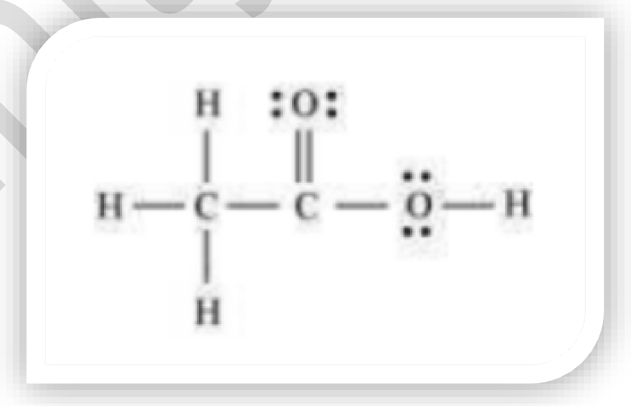
$N2 < SO2 < ClF3 < K2O < LiF.$

4.20 The skeletal structure of CH_3COOH as shown below is correct, but some of the bonds are shown incorrectly. Write the correct Lewis structure for acetic acid.



Answer:

The accurate Lewis shape for acetic acid is as follows:



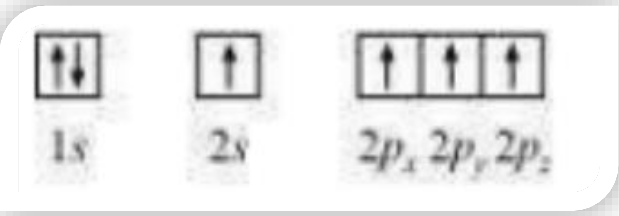
4.21 Apart from tetrahedral geometry, another possible geometry for CH_4 is square planar with the four H atoms at the corners of the square and the C atom at its centre. Explain why CH_4 is not square planar?

Answer:

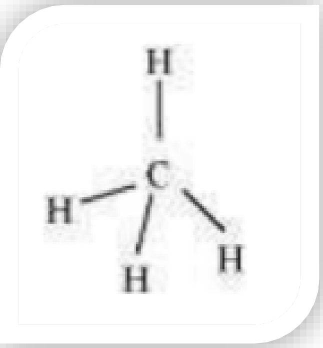
Electronic configuration of carbon atom:

${}_6C: 1s^2\ 2s^2\ 2p^2$

In the excited state, the orbital photograph of carbon may be represented as:



Hence, carbon atom undergoes sp^3 hybridization in CH_4 molecule and takes a tetrahedral shape.



For a rectangular planar shape, the hybridization of the primary atom needs to be dsp^2.

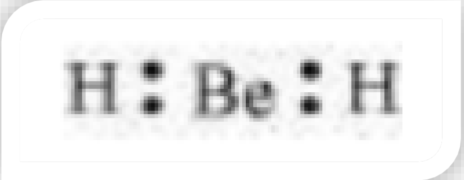
However, an atom of carbon does now no longer have d-orbitals to go through dsp^2 hybridization. Hence, the shape of CH_4 can't be rectangular planar.

Moreover, with a bond attitude of $90°$ in rectangular planar, the steadiness of CH_4 can be very much less due to the repulsion present among the bond pairs. Hence, VSEPR concept additionally helps a tetrahedral shape for CH_4.

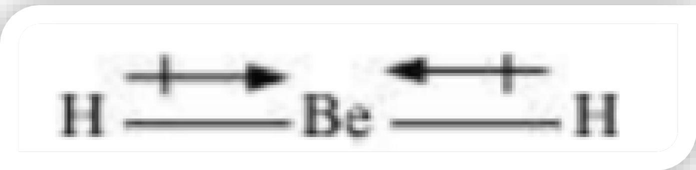
4.22 Explain why $\mathbf{BeH_2}$ molecule has a zero-dipole moment although the $\mathbf{Be-H}$ bonds are polar.

Answer:

The Lewis shape for $\mathbf{BeH_2}$ is as follows:



There isn't any any lone pair on the primary atom (Be) and there are bond pairs. Hence, $\mathbf{BeH_2}$ is of the sort AB_2. It has a linear structure.



Dipole moments of every $H-Be$ bond are same and are in contrary directions. Therefore, they nullify every other. Hence, $\mathbf{BeH_2}$ molecule has 0 dipole moment.

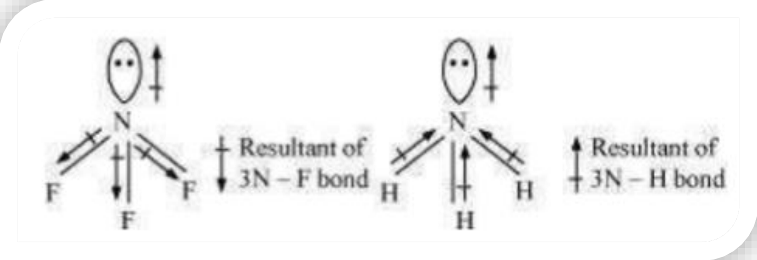
4.23 Which out of $\mathbf{NH_3}$ and $\mathbf{NF_3}$ has higher dipole moment and why?

Answer:

In each molecules i.e., NH_3 and NF_3, the valuable atom (N) has a lone pair electron and there are 3 bond pairs. Hence, each molecules have a pyramidal shape. Since fluorine is extra electronegative than hydrogen, its miles anticipated that the internet dipole second of NF_3 is more than NH_3. However, the internet dipole second of NH_3 $(1.46$ D) is more than that of NF_3 $(0.24$ D).

$\left(and \left(and \left(and \right)\right)\right)$

This may be defined on the idea of the guidelines of the dipole moments of every person bond in NF_3 and NH_3. These guidelines may be proven as:



Thus, the ensuing second of the $N-H$ bonds upload as much as the bond second of the lone pair (the 2 being withinside the identical direction), while that of the 3 $N - F$ bonds in part cancels the instant of the lone pair.

Hence, the internet dipole second of NF_3 is much less than that of NH_3.

4.24 What is meant by hybridisation of atomic orbitals? Describe the shapes of $\mathbf{sp}$, $\mathbf{sp^2}$, $\mathbf{sp^3}$ hybrid orbitals.

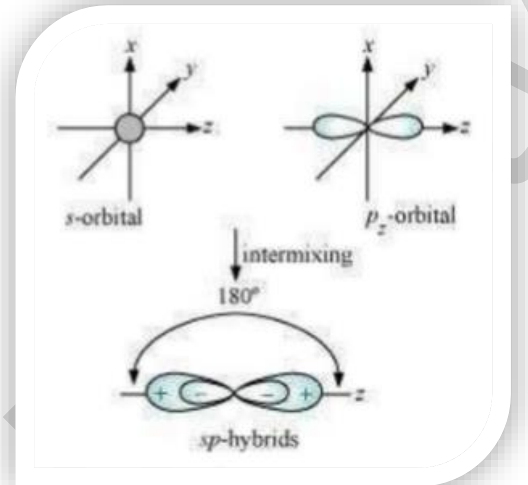
Answer:

Hybridization is described as an intermixing of a hard and fast of atomic orbitals of barely distinct energies, thereby forming a brand new set of orbitals having equal energies and shapes.

For example, one $2s-$orbitals hybridizes with $2p-$orbitals of carbon to shape 3 new sp^2 hybrid orbitals.

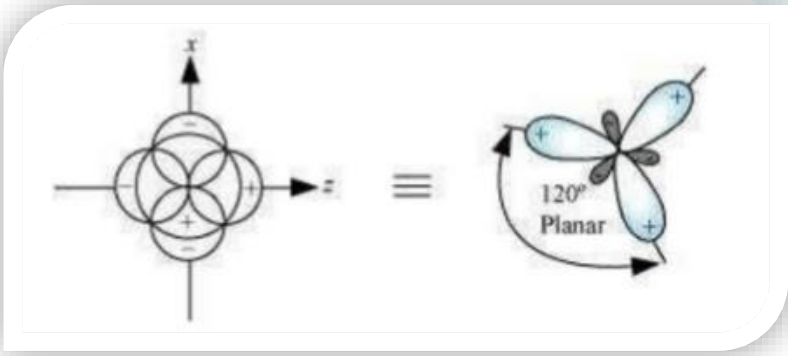
These hybrid orbitals have minimal repulsion among their electron pairs and thus, are extra stable. Hybridization allows imply the geometry of the molecule.

Shape of **sp** hybrid orbitals: sp hybrid orbitals have a linear shape. They are fashioned with the useful resource of the use of the intermixing of s and p orbitals as:



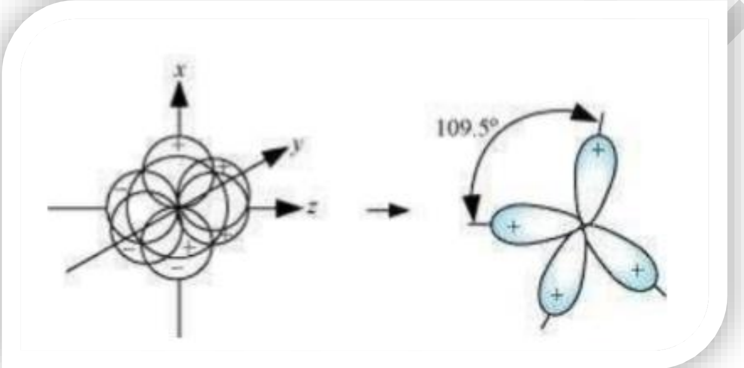
Shape of sp^2 hybrid orbitals:

sp^2 hybrid orbitals are shaped because of the intermixing of 1 s-orbital and $2p$ orbitals. The hybrid orbitals are orientated in a trigonal planar association as:



Shape of $\mathbf{sp^3}$ hybrid orbitals:

Four sp^3 hybrid orbitals are fashioned with the aid of using intermixing one s-orbital with 3 p-orbitals. The 4 sp^3 hybrid orbitals are organized withinside the shape of a tetrahedron as:

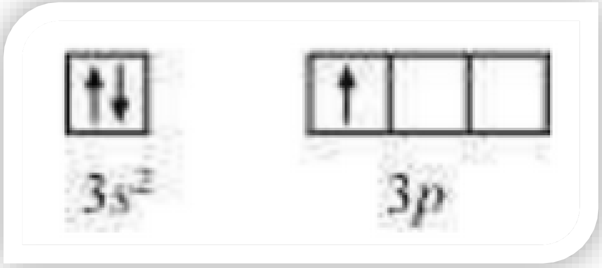


4.25 Describe the change in hybridization (if any) of the Al atom in the following reaction.

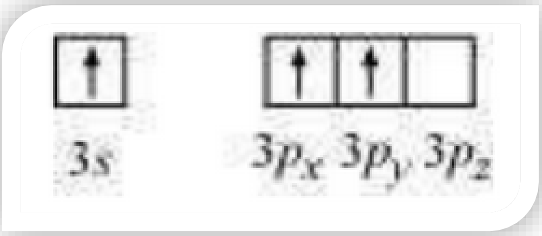
$AlCl_3 + Cl^- \rightarrow AlCl_4^-$

Answer:

The valence orbital image of aluminium withinside the floor country may be represented as:



The orbital image of aluminium withinside the excited nation may be represented as:



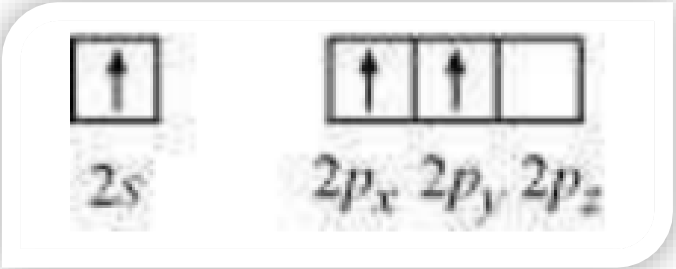
Hence, it undergoes sp^2 hybridization to present a trigonal planar arrangement (in $AlCl_3$). To shape $AlCl_4^-$, the empty $3p_z$ orbital additionally receives worried and the hybridization modifications from sp^2 to sp^3. As a result, the form receives modified to tetrahedral.

4.26 Is there any change in the hybridisation of B and N atoms as a result of the following reaction?

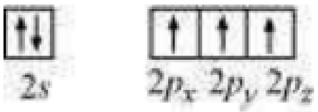
$\mathbf{BF_3 + NH_3 \rightarrow F_3B.NH_3}$

Answer:

Boron atom in BF_3 is sp^2 hybridized. The orbital photograph of boron withinside the excited kingdom can be proven as:



Nitrogen atom in NH_3 is sp^3 hybridized. The orbital photo of nitrogen may be represented as:



After the response has occurred, an adduct $F_3B.NH_3$ is fashioned as hybridization of 'B' adjustments to sp^3. However, the hybridization of 'N' stays intact.

4.27 Draw diagrams showing the formation of a double bond and a triple bond between carbon atoms in $\mathrm{C_2H_4}$ and $\mathrm{C_2H_2}$ molecules.

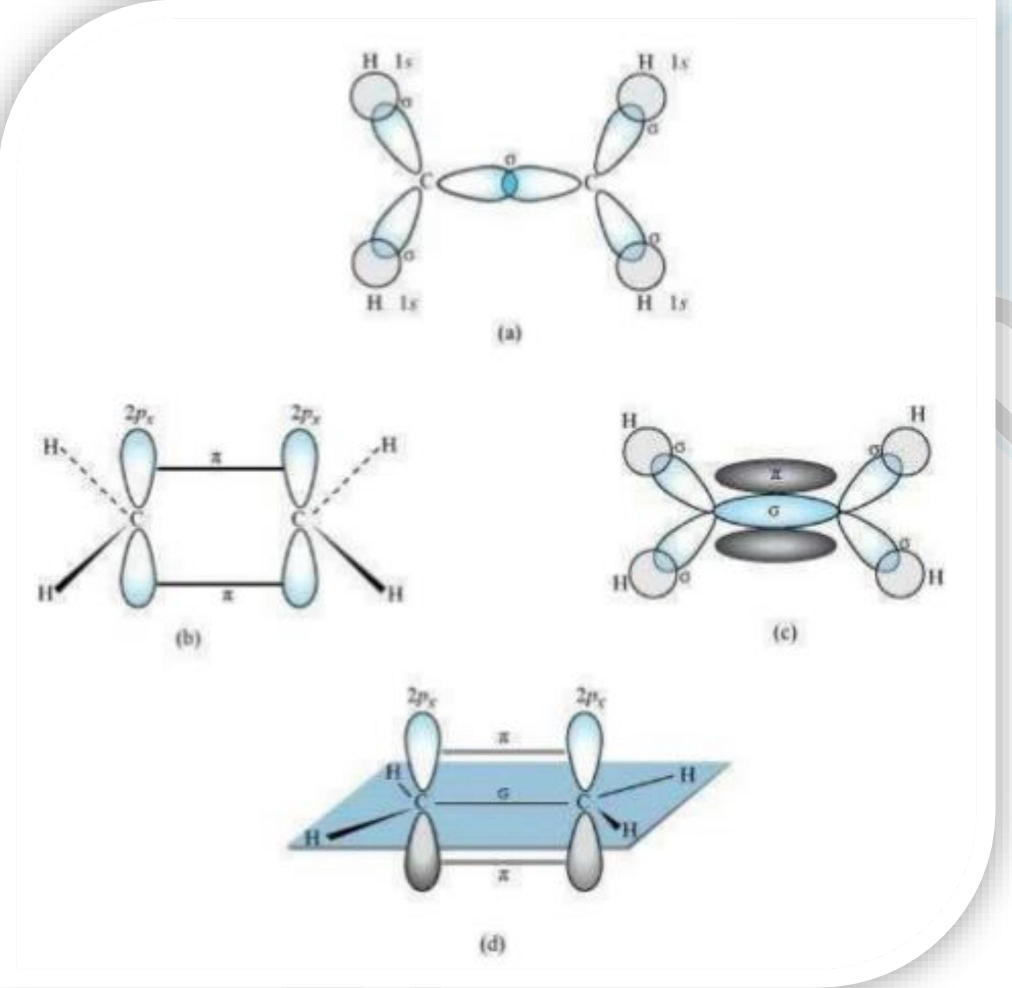
Answer:

$\mathrm{C_2H_4}$:

The digital configuration of $C-$atom withinside the excited kingdom is:

$${}_6C = 1s^2\, 2s^1\, 2p_x^1\, 2p_y^1\, 2p_z^1$$

In the formation of an ethane molecule (C_2H_4), one sp^2 hybrid orbital of carbon overlaps a sp^2 hybridized orbital of every other carbon atom, thereby forming a $C-C$ sigma bond. The final sp^2 orbitals of every carbon atom shape a sp^2-s sigma bond with hydrogen atoms. The unhybridized orbital of 1 carbon atom undergoes sidewise overlap with the orbital of a comparable type gift on every other carbon atom to shape a vulnerable $\pi-$bond.



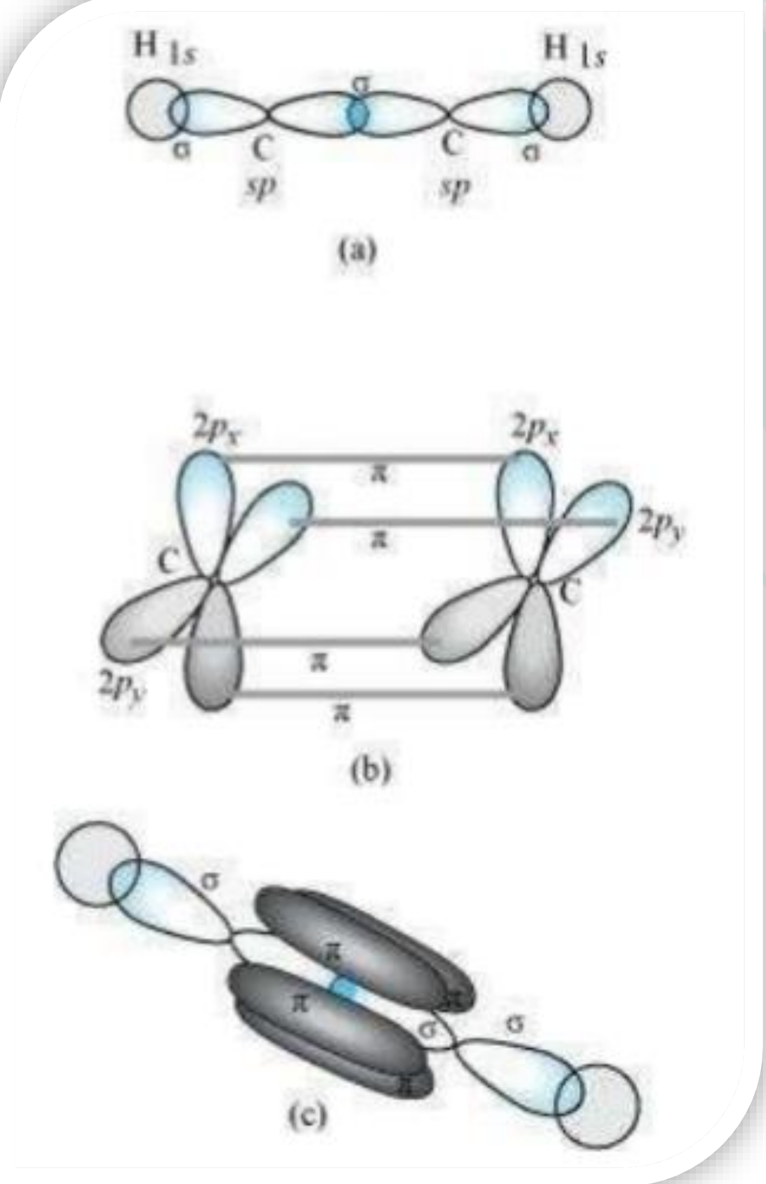
C_2H_2 :

In the formation of C_2H_2 molecule, every $C-$atom is sp hybridized with $2p-$orbitals in an unhybridized state.

One sp orbital of every carbon atom overlaps with the alternative alongside the internuclear axis forming a $C-C$ sigma bond. The 2nd sp orbital of every $C-$atom overlaps a half-stuffed $1s-$orbital to shape a σ bond.

The unhybridized $2p-$orbitals of the primary carbon go through sidewise overlap with the $2p-$orbital of every other carbon atom, thereby forming pi (π) bonds among carbon atoms.

Hence, the triple bond among carbon atoms is made up of 1 sigma and $\pi-$bonds.



4.28 What is the total number of sigma and pi bonds in the following molecules?

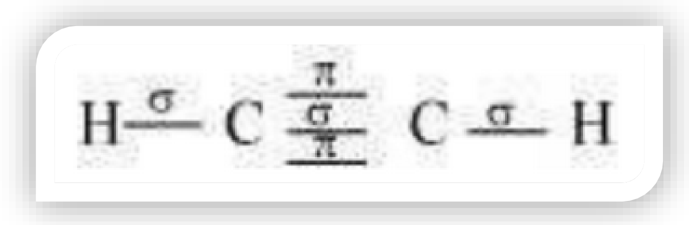
(a) $\mathbf{C_2H_2}$

(b) $\mathbf{C_2H_4}$

Answer:

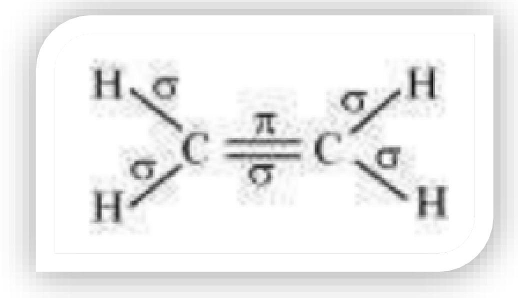
A single bond is a end result of the axial overlap of bonding orbitals. Hence, it contributes a sigma bond. A more than one bond (double or triple bond) is constantly fashioned due to the sidewise overlap of orbitals. A $\pi-$bond is constantly found in it. A triple bond is a mixture of $\pi-$bonds and one sigma bond.

Structure of C_2H_2 may be represented as:



Hence, there are 3 sigma and pi-bonds in C_2H_2.

The structure of C_2H_4 may be represented as:



Hence, there are 5 sigma and pi-bonds in C_2H_4.

4.29 Considering x – axis as the internuclear axis which out of the following will not form a sigma bond and why?

(a) 1s and 1s (b) 1s and 2px (c) 2py and 2py (d) 1s and 2s.

Answer:

$2py$ and $2py$ orbitals will now no longer a shape a sigma bond. Taking $x-$ axis because the internuclear axis, $2py$ and $2py$ orbitals will go through lateral overlapping, thereby forming a pi (π) bond.

4.30 Which hybrid orbitals are used by carbon atoms in the following molecules?

(a) $\mathbf{CH_3-CH_3}$;

(b) $\mathbf{CH_3-CH=CH_2}$;

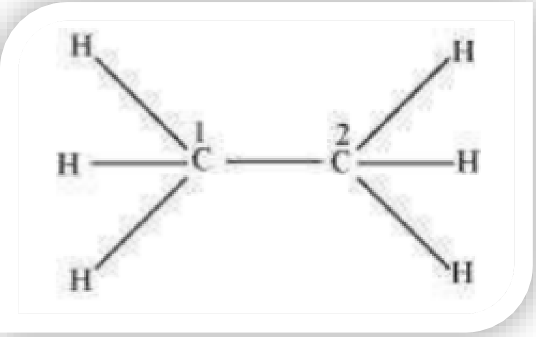
(c) $\mathbf{CH_3-CH_2-OH}$;

(d) $\mathbf{CH_3-CHO}$;

(e) **CH_3COOH**

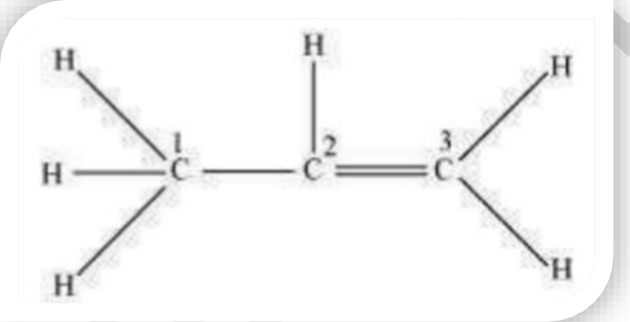
Answer:

(a)



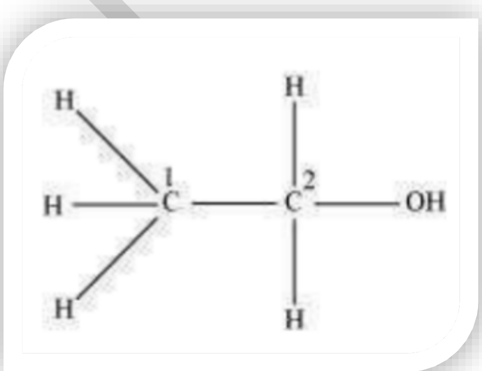
Both C_1 and C_2 are sp^3 hybridized.

(b)



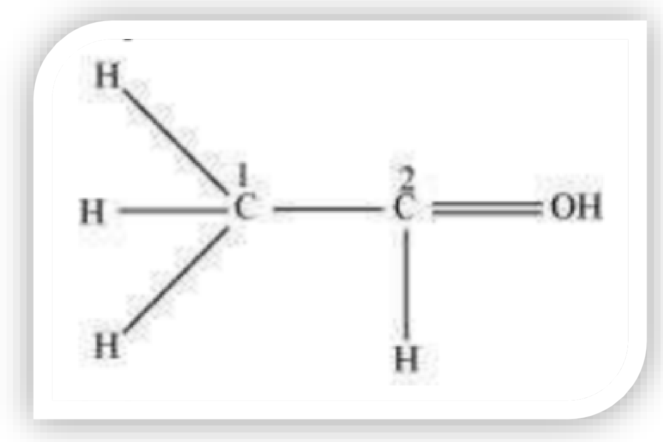
C_1 is sp^3 hybridized, at the same time as C_2 and C_3 are sp_2 hybridized.

(c)



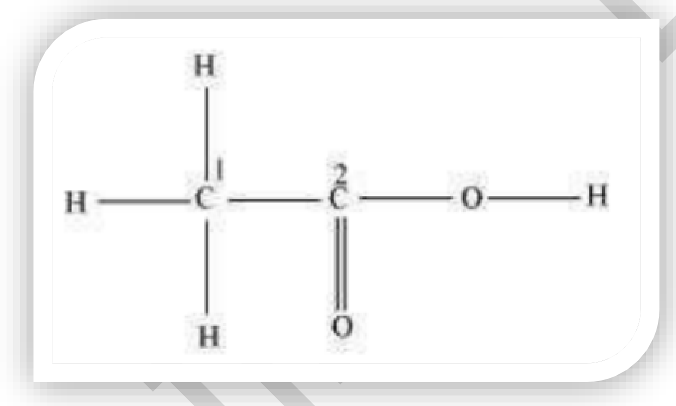
Both C_1 and C_2 are sp^3 hybridized.

(d)



C_1 is sp^3 hybridized and C_2 is sp_2 hybridized.

(e)



C_1 is sp^3 hybridized and C_2 is sp_2 hybridized.

4.31 What do you understand by bond pairs and lone pairs of electrons? Illustrate by giving one example of each type.

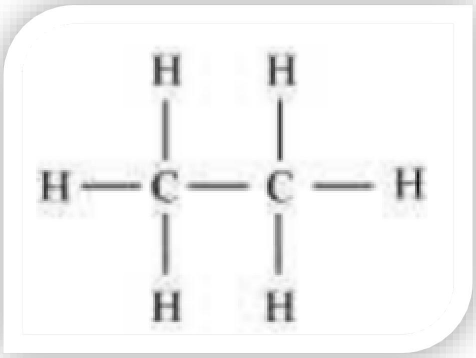
Answer:

A covalent connection is created between two atoms when they share one or more of their valence electrons.

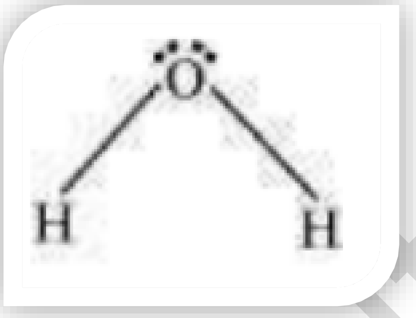
Bond pairs are the shared pairs of electrons that exist between bound atoms.

Bonding does not require the participation of all valence electrons. Lone pairs of electrons are electron pairs that do not engage in bonding.

For example, in C_2H_6 (ethane), there are seven bond pairs but no lone pair present.



In H_2O, there are bond pairs and lone pairs at the vital atom (oxygen).



4.32 Distinguish between a sigma and a pi bond.

Answer:

Sigma (σ) Bond	**Pi (π) Bond**
(a) It is made up of orbitals that overlap from end to end.	(a) The lateral overlap of orbitals creates it.
(b) The orbitals involved in the overlapping are $s-s$, $s-p$, or $p-p$.	(b) $s-s$, $s-p$, and $p-p$ orbitals are implicated in the overlapping.
(c) It's a strong connection.	(c) It's a weak connection
(d) Around the line connecting the two nuclei, the electron cloud is symmetrical.	(d) The electron cloud isn't even close to being symmetrical.
(e) It is made up of a single symmetrical electron cloud around the internuclear axis.	(e) Above and below the plane of the atomic nucleus, there are two electron clouds.
(f) It is possible to rotate freely around bonds.	(f) In the case of pi-bonds, rotation is limited.

4.33 Explain the formation of H_2 molecule on the basis of valence bond theory.

Answer:

Consider two hydrogen atoms (A and B) with nuclei (N_A and N_B) and electrons (e_A and e_B) undergoing a process to form a hydrogen molecule.

There is no interaction between A and B when they are separated by a considerable distance.

The attracting and repulsive forces begin to work as they approach each other.

(a) One atom's nucleus and its own electron, i.e., $N_A - e_A$ and $N_B - e_B$;

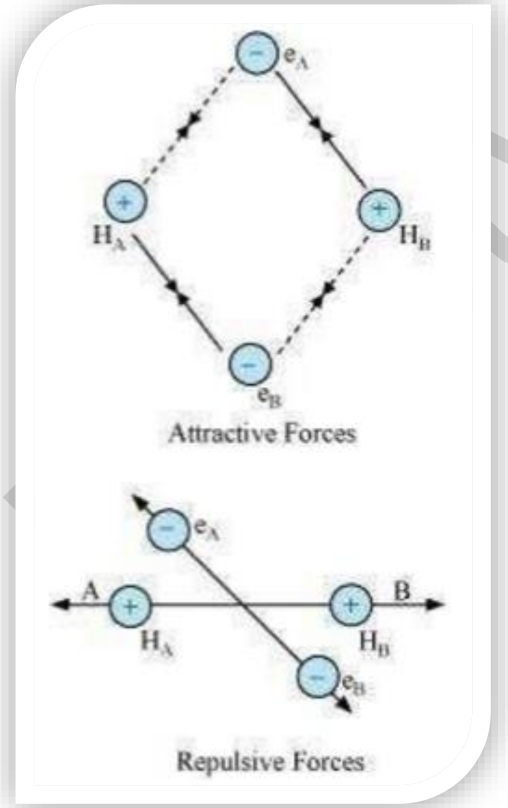
(b) One atom's nucleus and another atom's electron, i.e., $N_A - e_B$ and $N_B - e_A$.

Repulsive force exists between:

(a) Electrons of two atoms, $e_A - e_B$;

(b) Two-atom nuclei, such as $N_A - N_B$.

The attraction force pulls the two atoms together, while the repulsion force pushes them apart.



The attracting forces have a greater magnitude than the repulsive forces. As a result, the two atoms are approaching one other. As a result, the potential energy of the system is reduced. Finally, the system reaches a condition where the attracting and repulsive forces are balanced, and the system has the least amount of energy. A dihydrogen molecule is formed as a result of this reaction.

4.34 Write the important conditions required for the linear combination of atomic orbitals to form molecular orbitals.

Answer:

To generate molecular orbitals, atomic orbitals must satisfy the following conditions:

(a) The energy of the combining atomic orbitals must be the same or nearly so. This means that an atom's $1s-$atomic orbital can link with another atom's $1s-$atomic orbital in a homonuclear molecule, but not with the $2s-$orbital.

(b) To ensure maximal overlap, the combining atomic orbitals must be properly oriented.

(c) The amount of overlap should be substantial.

4.35 Use molecular orbital theory to explain why the $\mathbf{Be_2}$ molecule does not exist.

Answer:

Beryllium's electrical configuration is $1s^2\,2s^2$.

The electronic configuration of the molecular orbitals of the Be_2 molecule is written as:

$$\sigma_{1s}^{2}\,\sigma_{1s}^{\bullet 2}\,\sigma_{2s}^{2}\,\sigma_{2s}^{\bullet 2}$$

As a result, Be_2's bond order is $\frac{1}{2}(N_b - N_a)$

Where,

N_b = The number of electrons in the bonding orbitals is the number of electrons in the bonding orbitals.

N_a = Anti-bonding orbitals have a certain number of electrons.

$\therefore$ Bond order of $Be_2 = \frac{1}{2}$(4-4)=0

A molecule with a negative or zero bond order is unstable. As a result, the Be_2 molecule does not exist.

4.36 Compare the relative stability of the following species and indicate their magnetic properties;

$\mathbf{O_2, O_2^+, O_2^-}$ (superoxide), $\mathbf{O_2^{2-}}$ (peroxide).

Answer:

A molecule of dioxygen has 16 electrons, 8 from each oxygen atom. The following is the electrical configuration of an oxygen molecule:

$$[\sigma-(1s)]^2[\sigma^\bullet(1s)]^2[\sigma(2s)]^2[\sigma^\bullet(2s)]^2[\sigma(1p_z)]^2[\pi(2p_x)]^2[\pi(2p_y)]^2[\pi^\bullet(2p_x)]^1[\pi^\bullet(2p_y)]^1$$

The number of bonding electrons $=\ 8\ =\ N_b$ and the number of anti-bonding orbitals $=\ 4\ =\ N_a$ because each oxygen atom's $1s$ orbital is not involved in boding.

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

Bond order $=\frac{1}{2}(8-4)$

$=\ 2$

In the same way, $\mathbf{O_2^+}$'s electrical configuration can be expressed as:

$$KK[\sigma(2s)]^2[\sigma^{\bullet}(2s)]^2[\sigma(2p_z)]^2[\pi(2p_x)]^2[\pi(2p_y)]^2[\pi^{\bullet}(2p_x)]^1$$

$N_b\ =\ 8$

$N_a\ =\ 3$

Bond order of $\mathbf{O_2^+} = \frac{1}{2}(8-3)$

$=\ 2.5$

Electronic configuration of $\mathbf{O_2^-}$ ion will be:

$$KK[\sigma(2s)]^2[\sigma^{\bullet}(2s)]^2[\sigma(2p_z)]^2[\pi(2p_x)]^2[\pi(2p_y)]^2[\pi^{\bullet}(2p_x)]^2[\pi^{\bullet}(2p_y)]^1$$

$N_b\ =\ 8$

$N_a\ =\ 5$

Bond order of $\mathbf{O_2^-} = \frac{1}{2}(8-5)$

$=\ 1.5$

Electronic configuration of $\mathbf{O_2^{2-}}$ ion will be:

$$KK[\sigma(2s)]^2[\sigma^{\bullet}(2s)]^2[\sigma(2p_z)]^2[\pi(2p_x)]^2[\pi(2p_y)]^2[\pi^{\bullet}(2p_x)]^2[\pi^{\bullet}(2p_y)]^2$$

$N_b\ =\ 8$

$N_a\ =\ 6$

Bond order of $\mathbf{O_2^{2-}} = \frac{1}{2}(8-6)$

$=1$

Bond order is directly related to bond dissociation energy. As a result, the higher the bond order, the more stable the system. The order of stability is $O_2^+ > O_2 > O_2^- > O_2^{2-}$ on this premise.

4.37 Write the significance of a plus and a minus sign shown in representing the orbitals.

Answer:

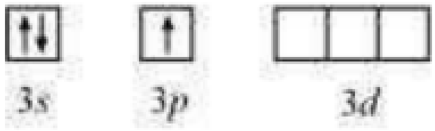
Wave functions are used to illustrate molecular orbitals. A positive wave function is represented by a plus sign in an orbital, while a negative wave function is represented by a minus sign in an orbital.

4.38 Describe the hybridisation in case of $\mathrm{PCl_5}$. Why are the axial bonds longer as compared to equatorial bonds?

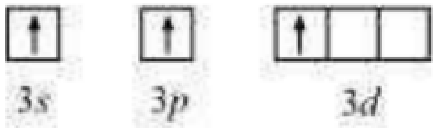
Answer:

The ground state and excited state outer electronic configurations of phosphorus $(Z = 15)$ are:

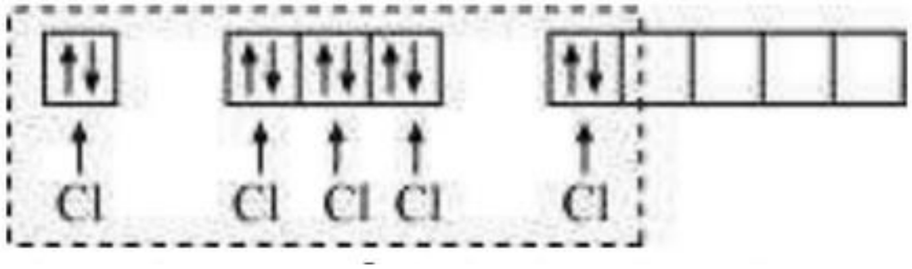
Ground state:



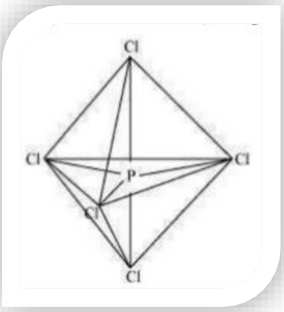
Excited state:



In the excited state, the phosphorus atom is sp^3d hybridized. The electron pairs given by five Cl atoms as PCl_5 fills these orbitals.



The five sp^3d hybrid orbitals are aimed at the trigonal bipyramidals' five corners. As a result, PCl_5's geometry can be represented as:



In PCl_5, there are five $P-Cl$ sigma bonds. Three $P-Cl$ bonds are arranged on a plane at a $120°$ angle to one another. Equatorial bonds are the name for these kind of bonds.

The remaining two $P-Cl$ bonds are 90 degrees apart and lie above and below the equatorial plane. Axial bonds are the name for these types of bonds.

Axial bonds are slightly longer than equatorial bonds because axial bond pairs are more repelled by equatorial bond pairs.

4.39 Define hydrogen bond. Is it weaker or stronger than the van der Waals forces?

Answer:

A hydrogen bond is described as an attractive force between hydrogen attached to one molecule's electronegative atom and hydrogen attached to another molecule's electronegative atom (may be of the same kind).

The bond pair between hydrogen and the electronegative atom drifts far away from the hydrogen atom due to a difference in electronegativities. As a result, a hydrogen atom gains a positive charge and becomes electropositive with regard to the other atom.

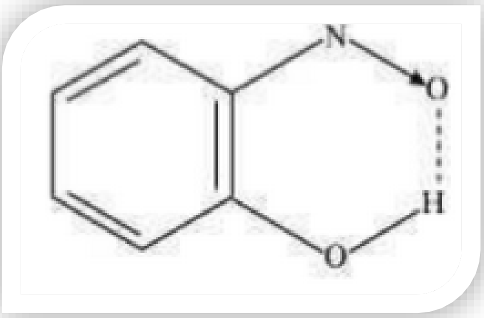
$$4^{\delta}-X^{\delta-}.....H^{\delta+}-X^{\delta-}.....H^{\delta+}-X^{\delta-}$$

In the solid state, $H-$bonding is greatest, while in the gaseous state, it is smallest.

$H-$bonds are divided into two types:

(i) Intermolecular $H-$bonds, such as HF and H_2O.

(ii) Intramolecular $H-$bonds, such as $o-$nitrophenol



Because hydrogen bonds are considered an extreme kind of dipole-dipole interaction, they are stronger than Van der Walls forces.

4.40 What is meant by the term bond order? Calculate the bond order of: N_2, O_2, O_2^+ and O_2^-

.

Answer:

One-half of the difference in the number of electrons present in the bonding and anti-bonding orbitals of a molecule is defined as bond order.

If the number of electrons in an anti-bonding orbital is equal to N_a, then the number of electrons in a bonding orbital is equal to N_b.

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

The molecule is believed to be stable if $N_b > N_a$.

If $N_b \leq N_a$, on the other hand, the molecule is deemed unstable.

The electrical configuration of N_2 can be used to compute the bond order:

$$[\sigma(1s)]^2[\sigma^{\bullet}(1s)]^2[\sigma(2s)]^2[\sigma^{\bullet}(2s)]^2[\pi(2p_x)]^2[\pi(2p_y)]^2[\sigma(2p_z)]^2$$

The number of bonding electrons is a measure of how strong a bond is., $N_b = 10$

Anti-bonding electrons are counted in the number of anti-bonding electrons., $N_a = 4$

The nitrogen molecule's bond order $= \frac{1}{2}(10-4)$

$= 3$

A dioxygen molecule has 16 electrons, eight from each oxygen atom. The following is the electrical configuration of an oxygen molecule:

$$[\sigma-(1s)]^2[\sigma^{\bullet}(1s)]^2[\sigma(2s)]^2[\sigma^{\bullet}(2s)]^2[\sigma(1p_z)]^2[\pi(2p_x)]^2[\pi(2p_y)]^2[\pi^{\bullet}(2p_x)]^1[\pi^{\bullet}(2p_y)]^1$$

The number of bonding electrons $= 8 = N_b$ and the number of anti-bonding electrons $= 4 = N_a$ because each oxygen atom's $1s$ orbital is not involved in boding.

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

$=\frac{1}{2}(8-4)$

$=2$

Hence, the bond order of oxygen molecule is 2.

In the same way, $\mathbf{O_2^+}$'s electrical configuration can be expressed as:

$$KK[\sigma(2s)]^2[\sigma^{\bullet}(2s)]^2[\sigma(2p_z)]^2[\pi(2p_x)]^2[\pi(2p_y)]^2[\pi^{\bullet}(2p_x)]^1$$

$N_b = 8$

$N_a = 3$

Bond order of $\mathbf{O_2^+}=\frac{1}{2}(8-3)$

$= 2.5$

Electronic configuration of $\mathbf{O_2^-}$ ion will be:

$$KK[\sigma(2s)]^2[\sigma^{\bullet}(2s)]^2[\sigma(2p_z)]^2[\pi(2p_x)]^2[\pi(2p_y)]^2[\pi^{\bullet}(2p_x)]^2[\pi^{\bullet}(2p_y)]^1$$

$N_b = 8$

$N_a = 5$

Bond order of $\mathbf{O_2^-}=\frac{1}{2}(8-5)$

$= 1.5$

As a result, the bond order of the ion $\mathbf{O_2^-}$ is $= 1.5$