

Chapter 4: Chemical Bonding and Molecular Structure

NCERT · Class 11 · Chemistry

Questions

Question 1

Explain the formation of a chemical bond.

Solution

“A chemical bond is an attractive force that bonds the constituents of a chemical species together.”

So many theories are suggested for chemical bond formation, such as valence shell electron pair repulsion theory, electronic theory, molecular orbital theory and valence bond theory.

The formation of a chemical bond is credited to the tendency of a system to achieve stability. It was noticed that the inertness of noble gases is the direct result of their completely filled outermost orbitals. Consequently, it was proposed that the elements having a deficiency of electrons in outermost shells are unstable. Thus, atoms combine with one another and finish their separate octets or duplets to achieve the stable configuration of the closest inert gases. So, this combination may occur either by sharing of electrons. The chemical bond formed as a result of sharing of electrons among atoms is known as a covalent bond. Also, an ionic bond is formed as a result of sharing of electrons among atoms.

Question 2

Write Lewis dot symbols for atoms of the following elements :

- a) Mg
- b) Na
- c) B
- d) O
- e) N

f) Br

Solution

a) Mg

The magnesium atom contains only 2 valence electrons. Thus, the Lewis dot symbols for Mg is



b) Na

The sodium atom contains only 1 valence electron. Thus, the Lewis dot symbol for Na is



c) B

The boron atom contains only 3 valence electrons. Thus, the Lewis dot symbols for B is



d) O

The oxygen atom contains only 6 valence electrons. Thus, the Lewis dot symbol for O is



e) N

The nitrogen atom contains only 5 valence electrons. Thus, the Lewis dot symbol for N is



f) Br

The bromine atom contains only 7 valence electrons. Thus, the Lewis dot symbols for Br is



Question 3

Write Lewis symbols for the following atoms and ions:

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

Solution

For S and S^{2-}

The sulphur atom contains only 6 valence electrons. Thus, the Lewis dot symbol for S is



The bi-negative charge on sulphur indicates that it has gained 2 electrons. So, there are six valence electrons plus two gained electrons.

Thus the Lewis dot symbol is



For Al and Al^{3+}

An aluminium atom contains only 3 valence electrons. Thus, the Lewis dot symbols for Al is



The tri-positive charge on aluminium indicates that it has donated 3 electrons.

Thus, the Lewis dot symbol is



For H and H^-

The hydrogen atom contains only 1 valence electron. Thus, the Lewis dot symbol for H is



The single negative charge on hydrogen indicates that it has gained 1 electron. So, one valance electron plus one gained electron.

Thus lewis dot symbol is



Question 4

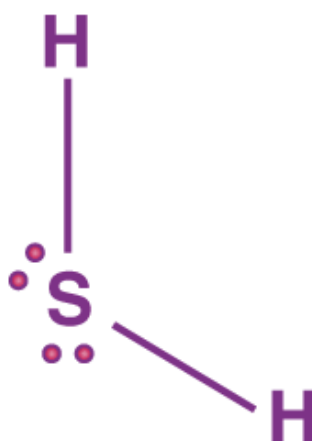
Draw the Lewis structures for the following molecules and ions :

H_2S , SiCl_4 , BeF_2 ,

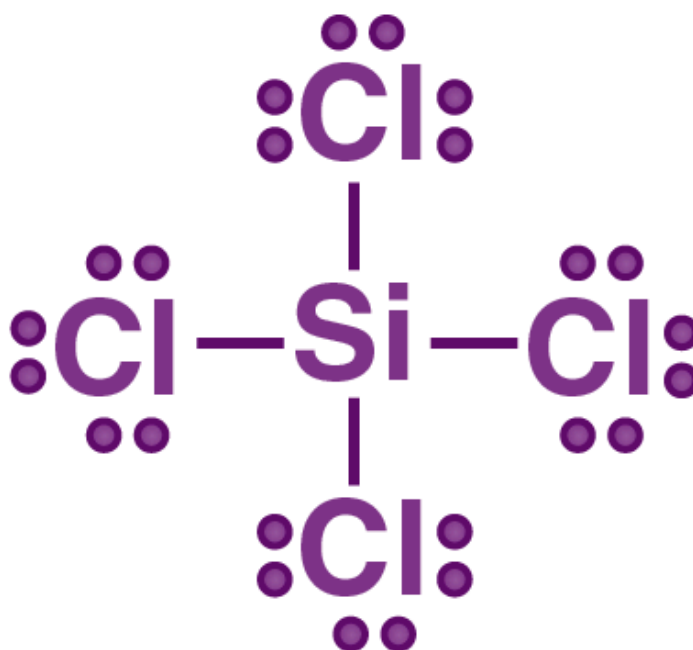
CO_3^{2-}
, HCOOH

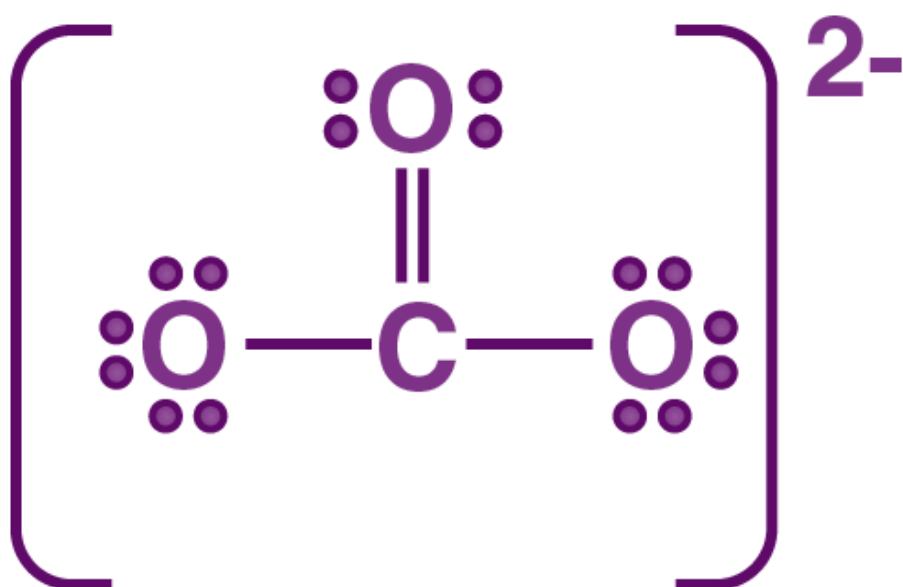
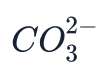
Solution

H_2S

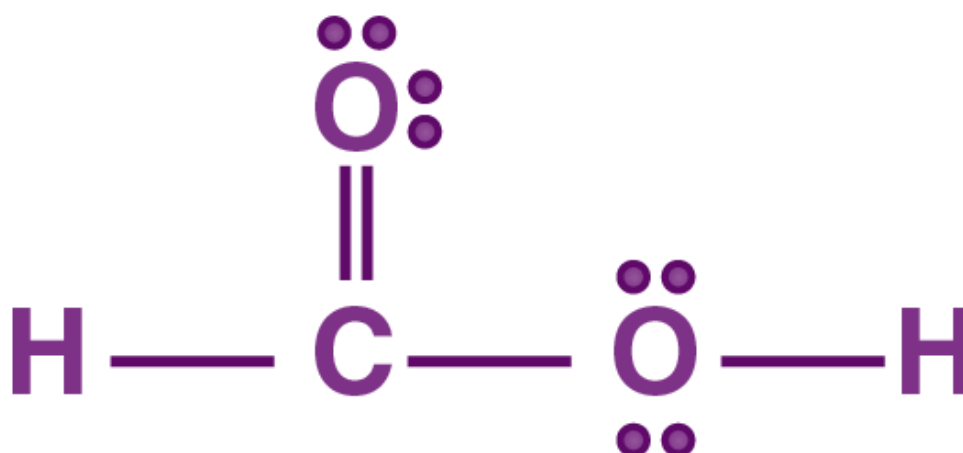


SiCl_4





Question 5



Define the octet rule. Write its significance and limitations.

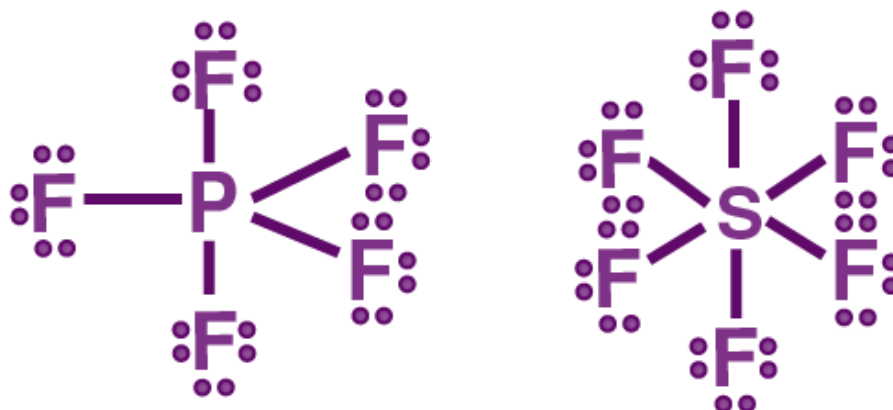
Solution

Octet rule says, “Atoms can combine either by transfer of valence electrons from one atom to another or by sharing their valence electrons in order to achieve the nearest inert gas configuration by having an octet in their valence shell.”

Octet rule explains chemical bond formation depending upon the nature of the element.

Limitations:

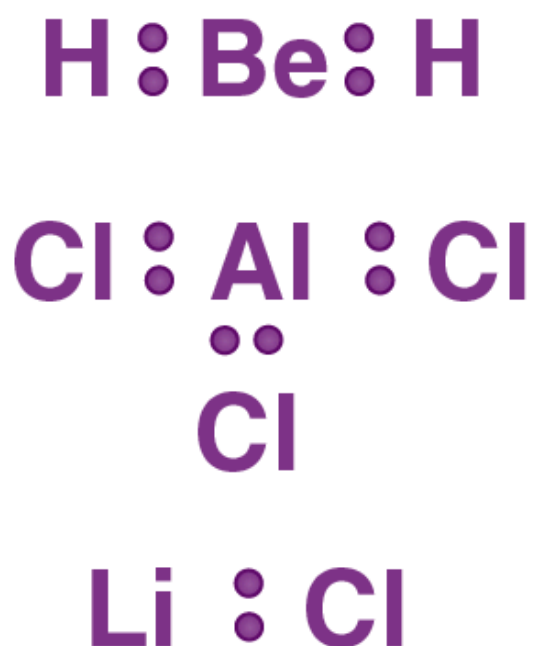
- (a) Octet rule fails to predict the relative stability and shape of the molecules.
- (b) It is based on the inert nature of noble gases. But, some inert gases, say krypton(Kr) and xenon(Xe), form compounds like KrF_2 , XeF_2 etc.
- (c) For elements beyond the 3rd period, the octet rule cannot be applied. Elements present beyond the 3rd period have more than 8 valence electrons surrounding the central atom. E.g. SF_6 , PF_6 etc.



(d) For atoms in a molecule having an odd number of electrons, the octet rule is not applied. E.g. For NO_2 and NO octet rule is not applicable.



(e) If a compound has less than 8 electrons surrounding the central atom, then the octet rule cannot be applied to that compound. E.g. BeH_2 , AlCl_3 , LiCl etc., does not obey the octet rule.



Question 6

Write the favourable factors for the formation of an ionic bond.

Solution

The formation of an ionic bond takes place through the transfer of 1 or more electrons from one atom to another. Thus, ionic bond formation depends on the flexibility of neutral atoms to lose or gain electrons. The formation of an ionic bond also depends on the lattice energy of the compound which is formed.

The factors that are favourable for ionic bond formation:

- (a) High electron affinity of atoms of non-metals.
- (b) The high lattice energy of the compound which is formed.
- (c) Low ionization enthalpy of an atom of metal.

Question 7

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

BeCl_2 , BCl_3 , SiCl_4 , AsF_5 , H_2S , PH_3

Solution

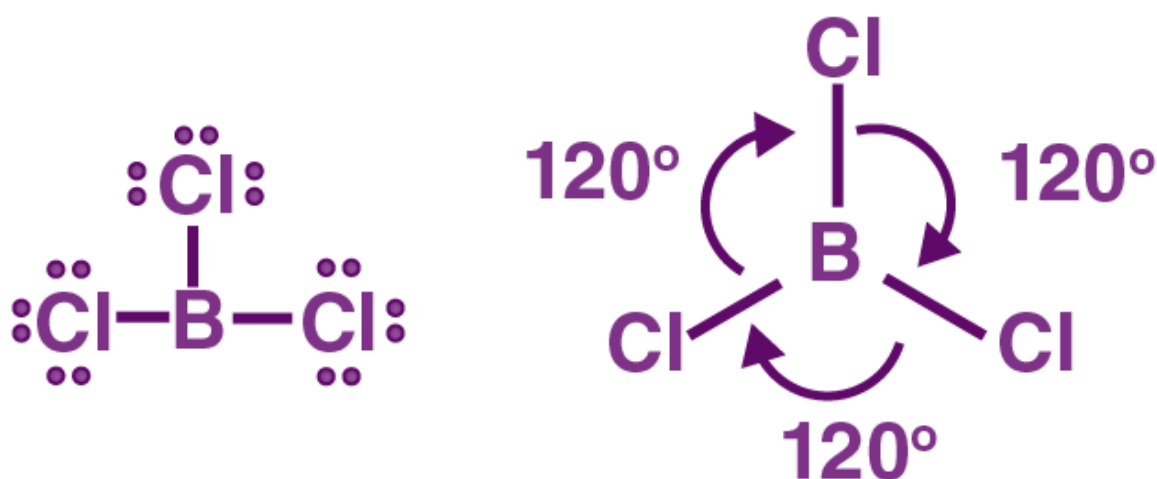
BeCl_2

The central atom does not have any lone pair but has 2 bond pairs. Thus, its shape is AB_2 , i.e., linear shape.

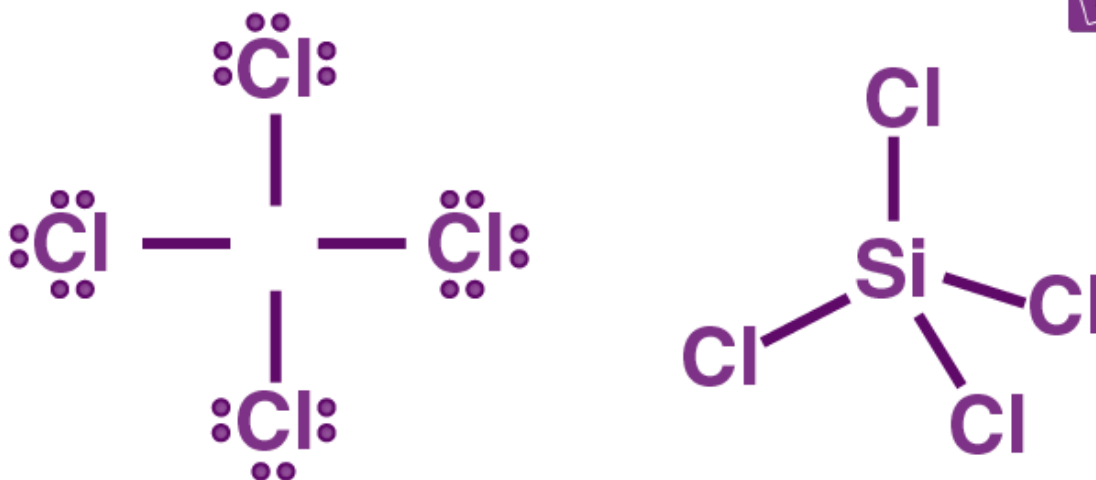


BCl_3

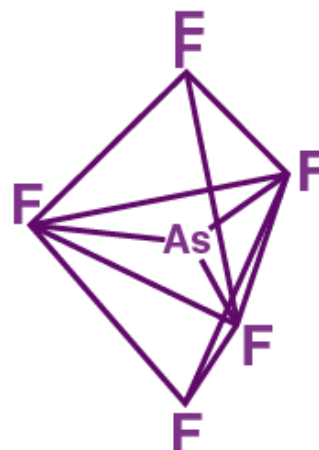
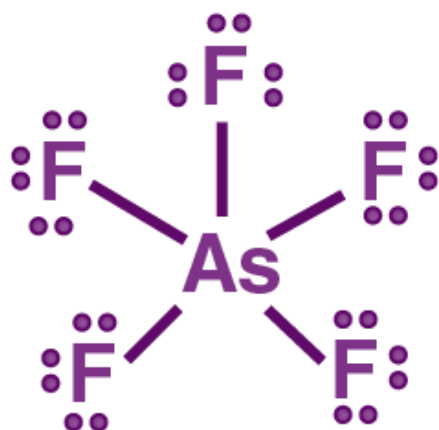
The central atom does not have any lone pair but has 3 bond pairs. Thus, its shape is AB_3 , i.e., trigonal planar.



The central atom does not have any lone pair but has 4 bond pairs. Thus, its shape is AB_4 , i.e., tetrahedral.



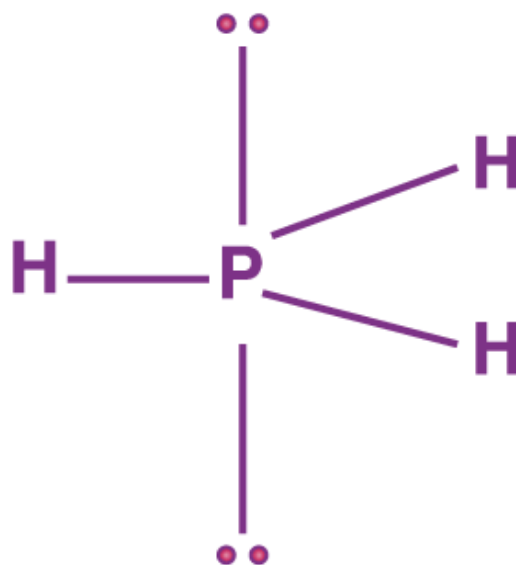
The central atom does not have any lone pair but has 5 bond pairs. Thus, its shape is AB_5 , i.e., trigonal bipyramidal.



The central atom has 1 lone pair and has 2 bond pairs. Thus, its shape is AB_2E , i.e., bent shape.



The central atom has 1 lone pair and has 3 bond pairs. Thus, its shape is AB_3E , i.e., trigonal bipyramidal.

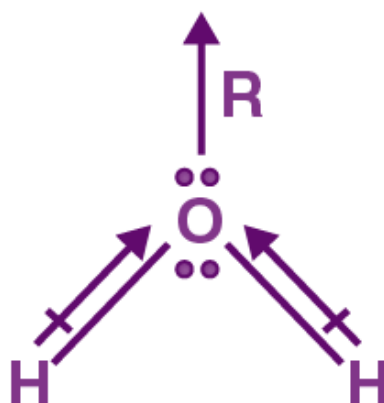


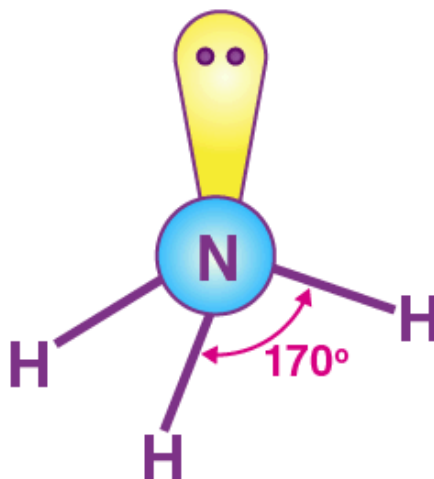
Question 8

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

Solution

The geometry of H_2O and NH_3 :





The central atom(N) in ammonia has 1 lone pair and has 3 bond pairs.

The central atom(O) in water has 2 lone pairs and has 2 bond pairs.

Thus, these 2 lone pairs on O- atom in the water molecule repels the 2 bond pairs. And this repulsion between the lone pair and the bond pair on O- atom of H_2O is stronger than the repulsion between the lone pair and bond pair on the N-atom of NH_3 .

Thus, the bond angle in H_2O is less than NH_3 , even though they have a distorted tetrahedral structure.

Question 9

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

Solution

The extent of bonding which occurs between two atoms while forming a molecule is represented by bond strength. As the bond strength increases, the bond becomes stronger, and the bond order increases.

Question 10

Define Bond length.

Solution

“Bond length is defined as the equilibrium distance between the nuclei of 2 bonded atoms in a molecule.”

Question 11

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

Solution

Experimental results shows that, all the C-O bond in



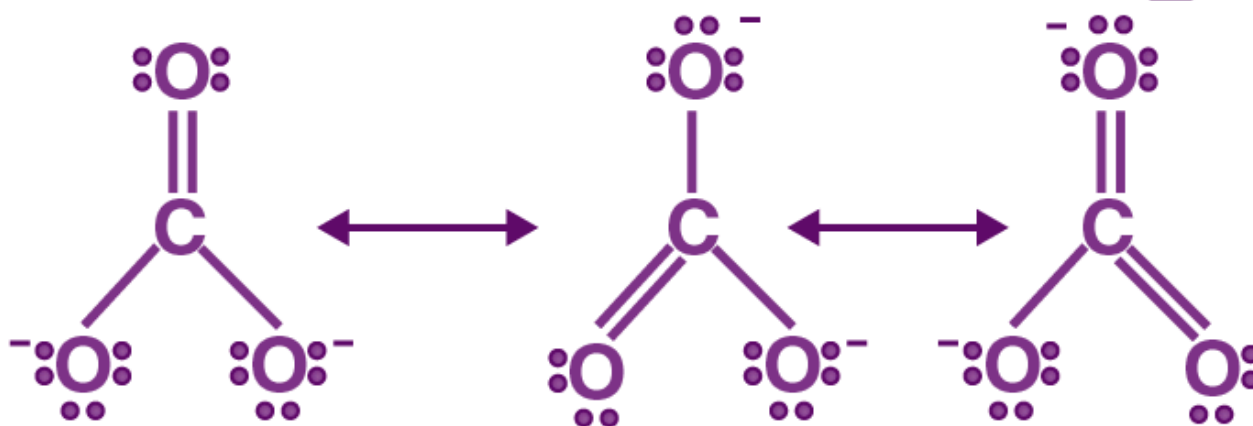
Thus, it is inefficient to represent



Thus, the resonance structures of



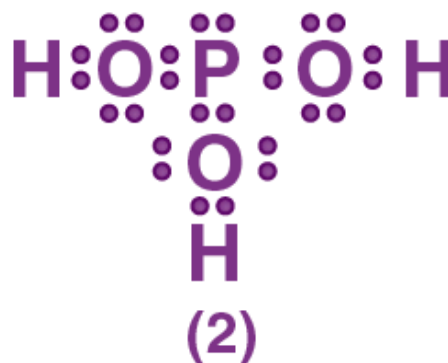
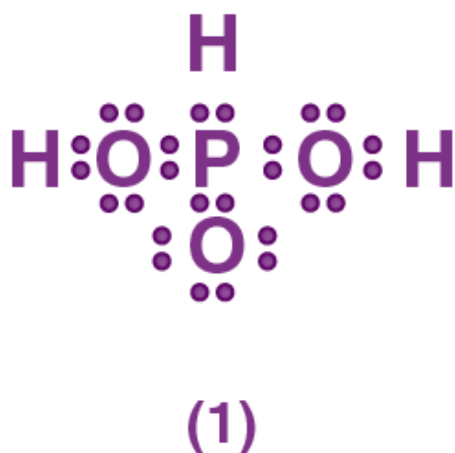
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Question 12

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.

Solution



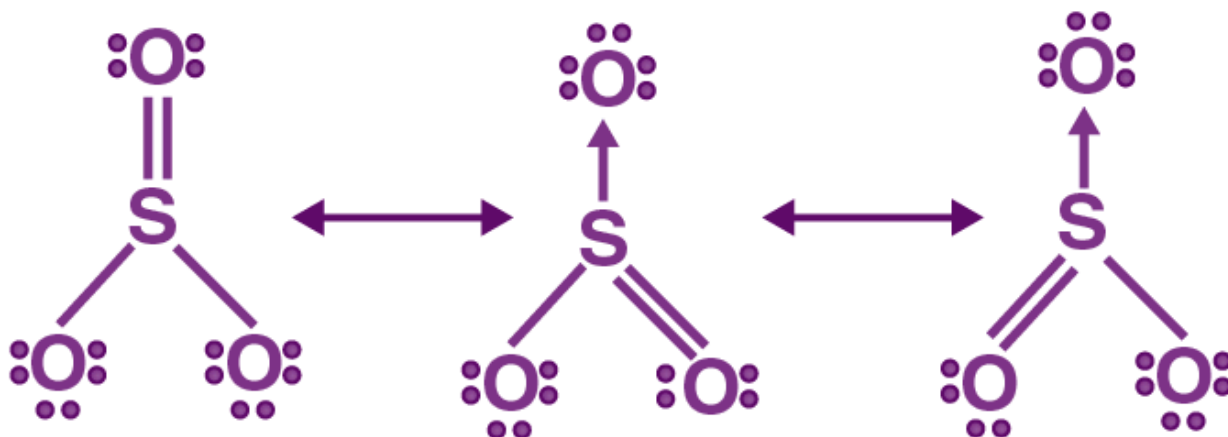
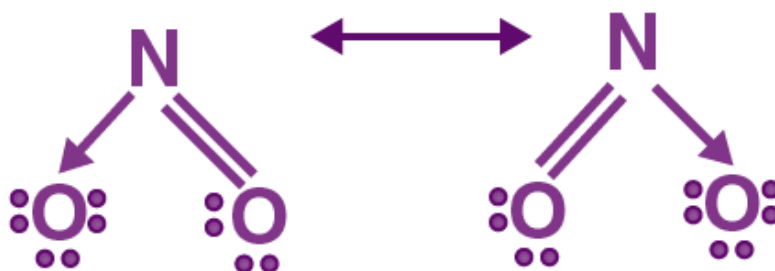
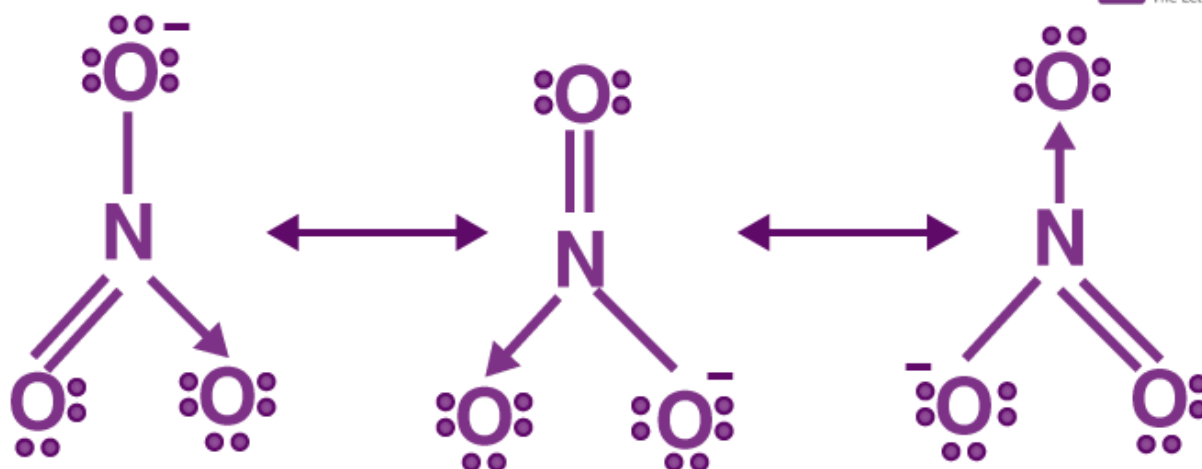
In the given structures, the position of atoms is changed, so we cannot take the 2 given structures as a canonical form of resonance hybrid which represents H_3PO_3 .

Question 13

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

Solution



 NO_2  NO_3^- 

Question 14

Use Lewis symbols to show electron transfer between the following atoms to form cations and anions :

(i) K and S

(ii) Ca and O

(iii) Al and N.

Solution

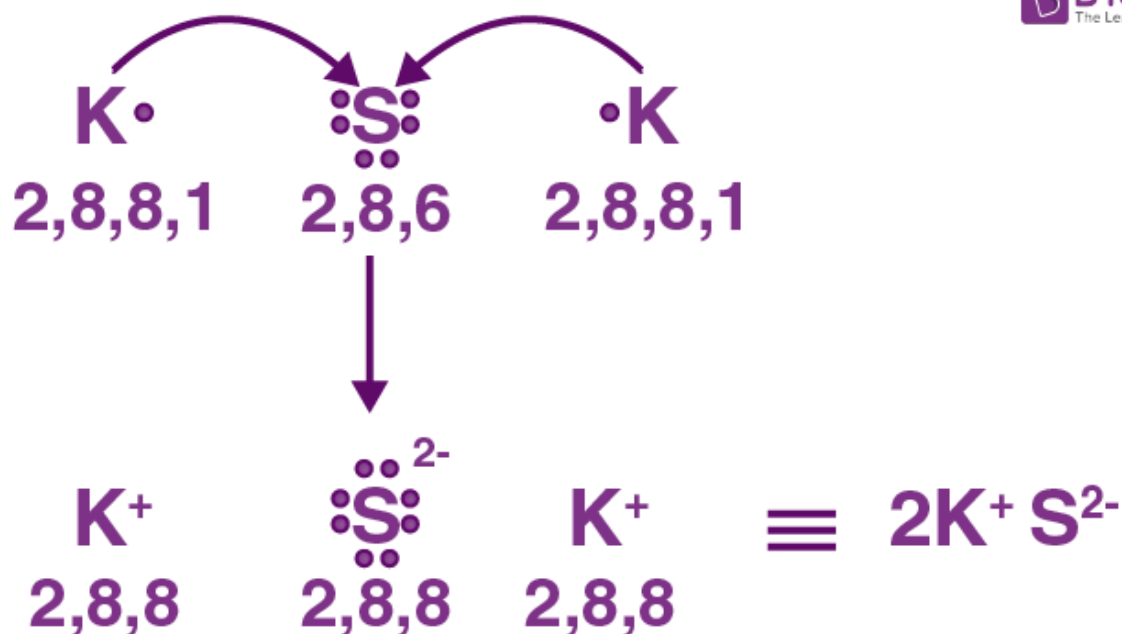
(i) K and S

Electronic configurations of S and K are:

S: 2, 8, 6

K: 2, 8, 8, 1

Here, it is clear that K has 1 more electron than the nearest inert gas, i.e., Ne, whereas S needs 2 electrons to complete its octet. Thus, the transfer of electrons takes place in the following way,



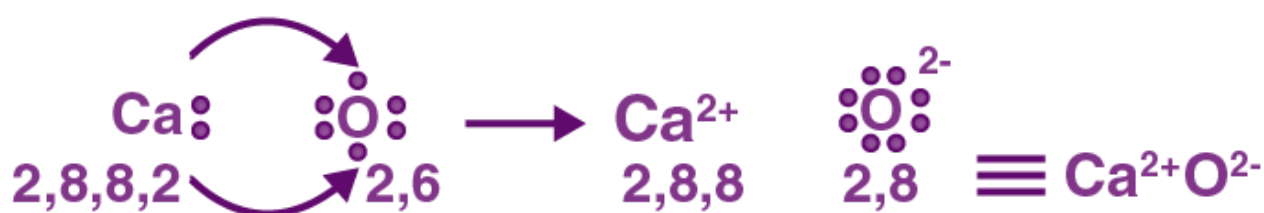
(ii) Ca and O

Electronic configurations of O and Ca are:

O: 2, 6

Ca: 2, 8, 8, 2

Here, it is clear that Ca has 2 more electrons than the nearest inert gas Ar, whereas O needs 2 electrons to complete its octet. Thus, the transfer of electrons takes place in the following way,



(iii) Al and N

Electronic configurations of N and Al are:

N: 2, 5

Al: 2, 8, 3

Here, it is clear that Al has 3 more electrons than the nearest inert gas Ne, whereas N needs 3 electrons to complete its octet. Thus, the transfer of electrons takes place in the following way,

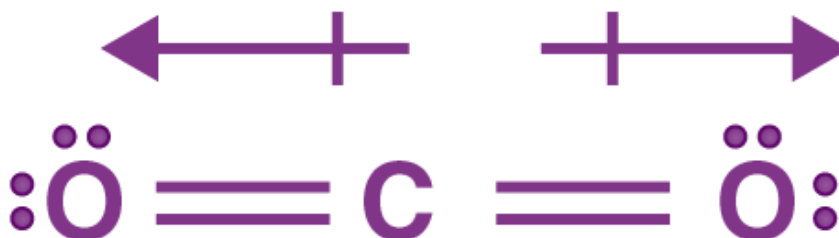


Question 15

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

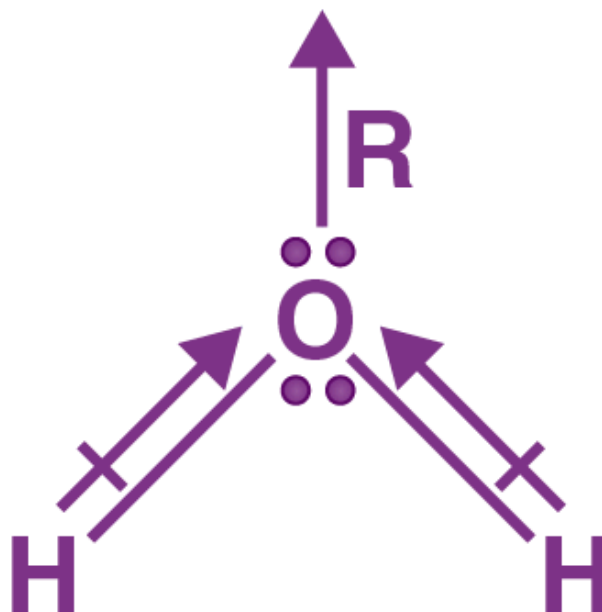
Solution

Experimental results show that the dipole moment of CO_2 is 0. And it is possible only if the shape of the molecule is linear as dipole moments of a bond between C-O are equal and opposite. So, it nullifies each other.



$\therefore$ Resultant, $\mu = 0$

H_2O has 1.84 D dipole moment. The value of dipole moments indicates that the structure of water molecule is bent as dipole moments of the bond between O-H are unequal.



Question 16

Write the significance/applications of dipole moment.

Solution

The following are some of the key significance of the dipole moment:

- The molecule's shape can be determined. Symmetrical molecules, such as linear, have zero dipole moments, whereas non-symmetrical molecules take on varied shapes, such as bent or angular.
- In order to determine the polarity of molecules. The polarity will be greater if the dipole moment is greater, and vice versa.
- We can say that if a molecule has zero dipole moment, it is non-polar, and if it has some polar character, it is non-polar.

Question 17

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

Solution

“Electronegativity is the ability of an atom in a chemical compound to attract a bond pair of electrons towards itself”.

Sr. No	Electronegativity	Electron affinity
1	A tendency to attract the shared pairs of electrons for an atom which is in a chemical compound is its electronegativity.	A tendency to gain electrons for an isolated gaseous atom is its electron gain enthalpy.
2	It varies according to the element with which it is bounded.	It does not vary according to the element with which it is bounded.
3	It is not constant for any element.	It is constant for an element.
4	It is not a measurable quantity.	It is a measurable quantity.

Question 18

Explain with the help of suitable example polar covalent bond.

Solution

When two unique atoms having distinct electronegativities join to form a covalent bond, the bond pair of electrons are not shared equally. The nucleus of an atom having greater electro-negativity attracts the bond pair. So, the electron distribution gets distorted and an electronegativity atom attracts the electron cloud.

Thus, the electronegative element gets slightly negatively charged and on the other hand, the other atom gets slightly positively charged. As a result of this, two opposite poles are developed in a molecule, and this type of bond formed is termed a ‘polar covalent bond’.

E.g. HCl is having a polar covalent bond. In HCl, Cl- atom has more electronegativity than H- atom. Thus, bond pair shifts towards Cl- atom and because of that, it acquires a positive charge.



Question 19

Arrange the bonds in order of increasing ionic character in the molecules: LiF, K₂O, N₂, SO₂, and ClF₃.

Solution

The ionic character of a molecule depends on the difference in electronegativity between constituents atoms. So, the higher the difference is, the higher the ionic character of a molecule will be.

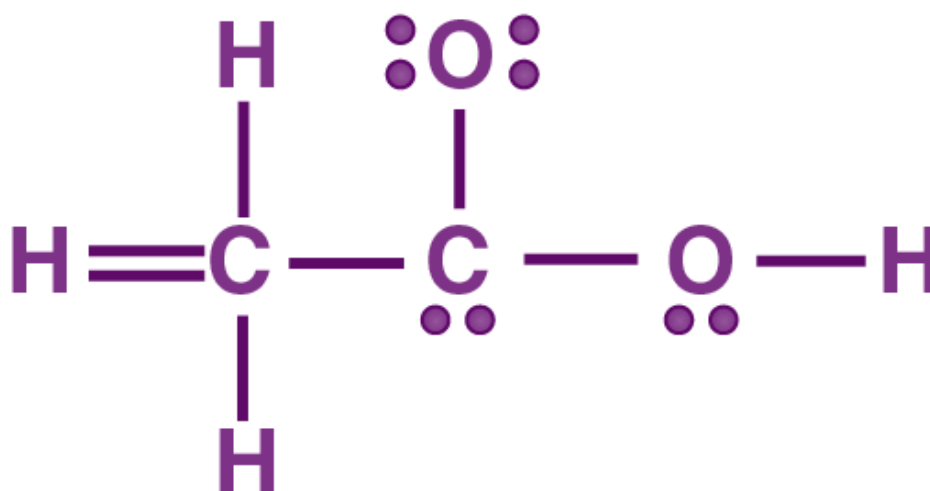
So, the required order of ionic character of the given molecules is



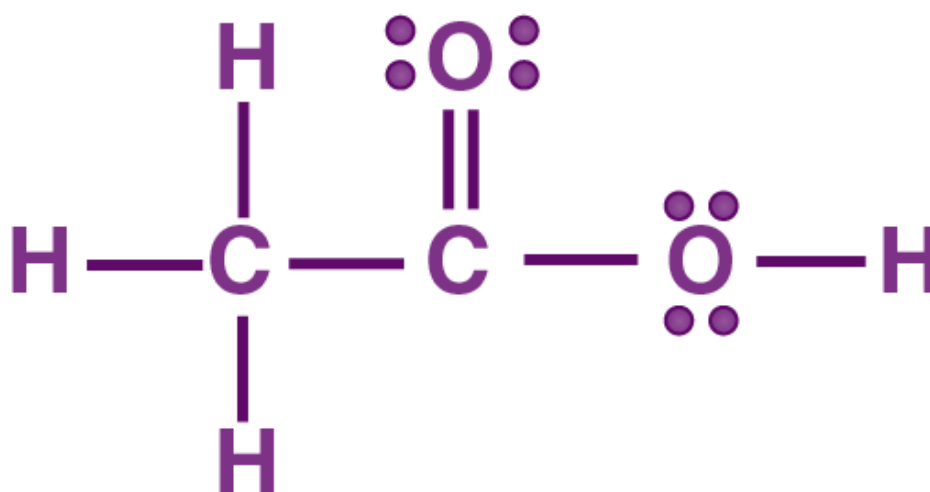
Question 20

The skeletal structure of CH₃COOH as shown below is correct, but some of the bonds are shown incorrectly. Write the correct Lewis structure for acetic acid.

Solution



Correct Lewis structure of CH_3COOH is given below:



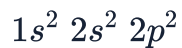
Question 21

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.

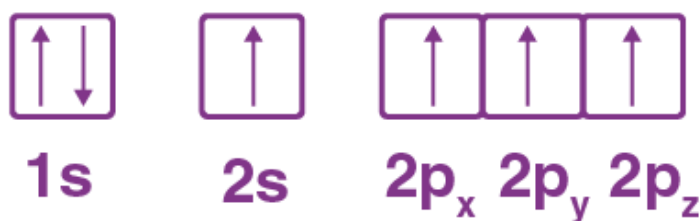
Solution

Electronic configuration of C- atom:

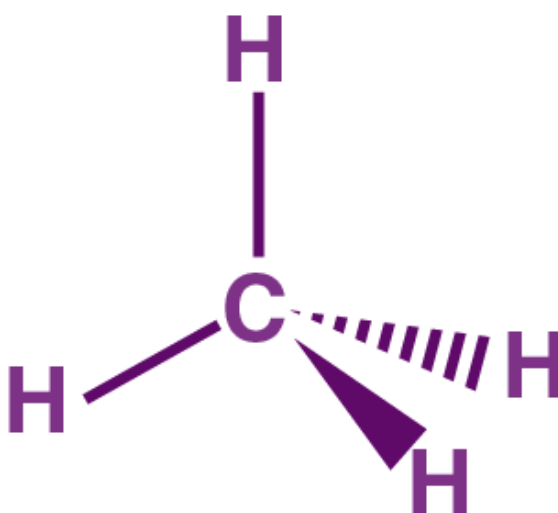
6C :



The orbital picture of C- atom in excited state is:



Thus, C- atom undergoes sp^3 hybridization in methane molecule and forms a tetrahedral structure.



For square planar geometry, C-atom should have dsp^2 hybridization. But as C- atom does not have a d-orbital, it cannot undergo dsp^2 hybridization. Thus, Methane's geometry cannot be square planar.

Also in square planar geometry the bond angle is

$$90^\circ$$

Question 22

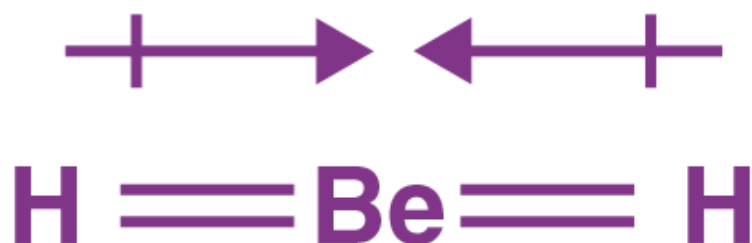
Explain why BeH_2 molecule has a zero dipole moment although the Be–H bonds are polar.

Solution

Lewis structure of BeH_2 is:



Central atom is not having any lone pair but has 2 bond pairs. Thus, its shape is AB_2 , i.e., linear shape.



Thus, the dipole moment of Be–H bond is equal and opposite in direction, nullifying one another. Thus, the dipole moment of BeH_2 is 0.

Question 23

Which out of NH_3 and NF_3 has higher dipole moment and why?

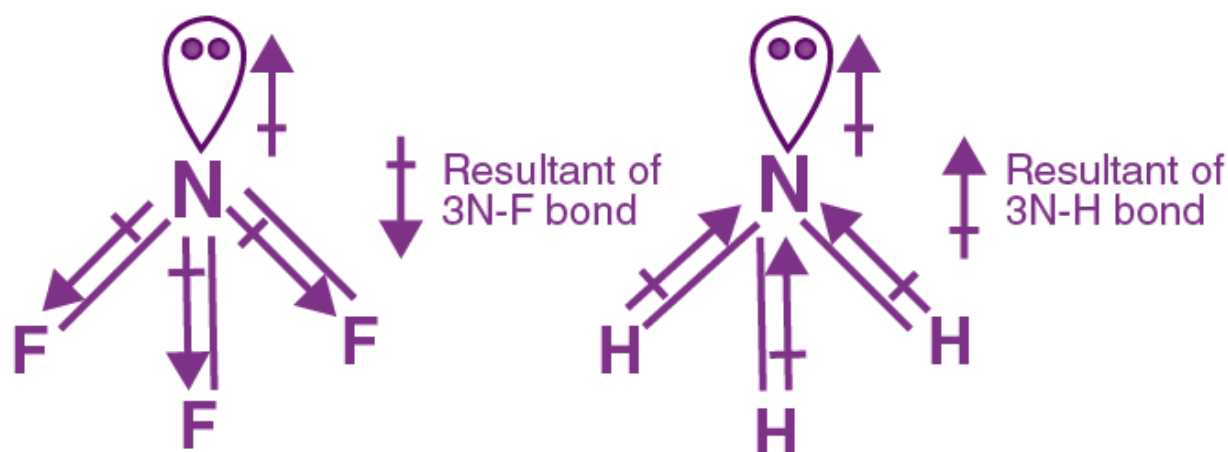
Solution

N- atom is the central atom of NF_3 and NH_3 .

Central atom has 1 lone pair and is having 3 bond pairs. Thus, for both, the shape is AB_3E , i.e., pyramidal.

As, the F-atom has more electronegativity than the H- atom, NF_3 should have a higher dipole moment than NH_3 . But the dipole moment of NH_3 is 1.46D which is higher than the dipole moment of NF_3 , which is 0.24D.

It gets clear from the directions of dipole moments of individual bonds in NF_3 and NH_3 .



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As both the N-H bonds are in the same direction, it adds to the bond moment of the lone pair, while N-F bonds are in the opposite direction. So they partly cut the bond moment of lone pair.

Thus, dipole moment of NH_3 is higher than that of NF_3 .

Question 24

What is meant by hybridisation of atomic orbitals? Describe the shapes of sp , sp^2 , sp^3 hybrid orbitals.

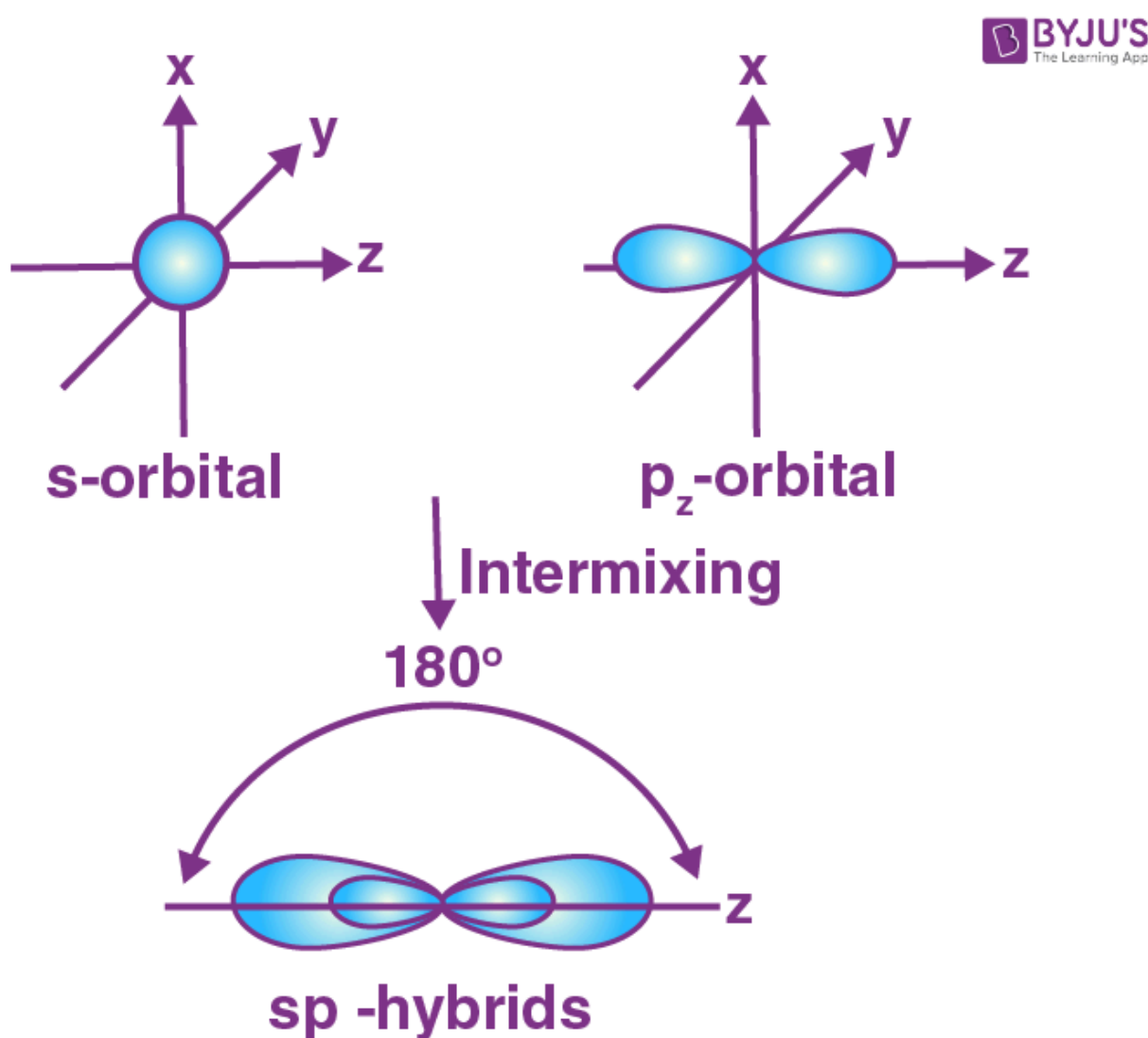
Solution

“Hybridization is defined as an intermixing of a set of atomic orbitals of slightly different energies, thereby forming a new set of orbitals having equivalent energies and shapes”.

E.g. 1 s- orbital hybridises with 3 p- orbitals to form 4 sp^3 hybrid orbitals.

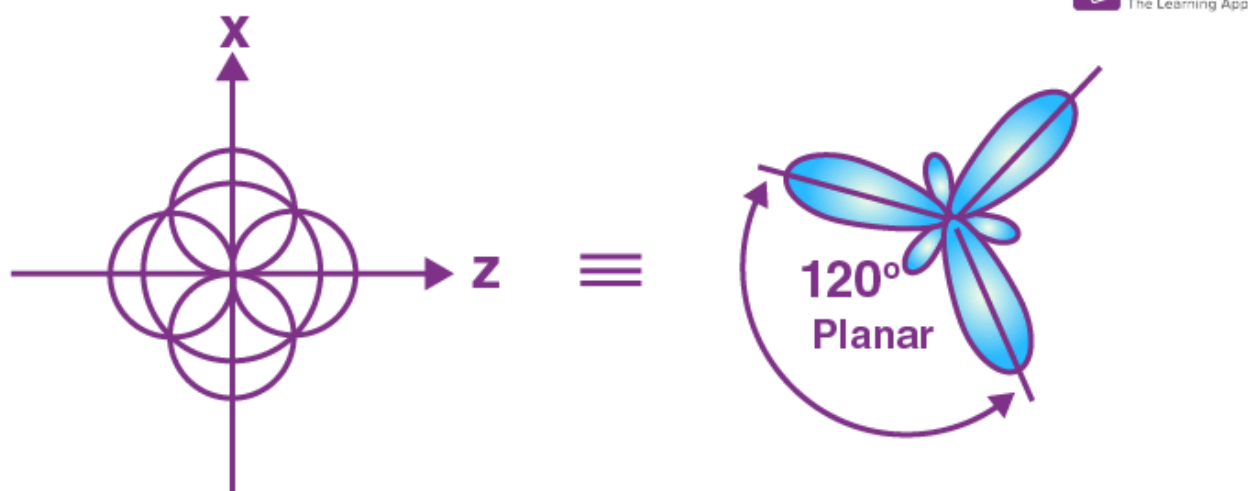
(a) sp hybrid orbital

1 s- orbital hybridises with 1 p- orbitals to form 2 sp hybrid orbitals. sp hybrid orbital has a linear shape. The formation of sp orbital is:



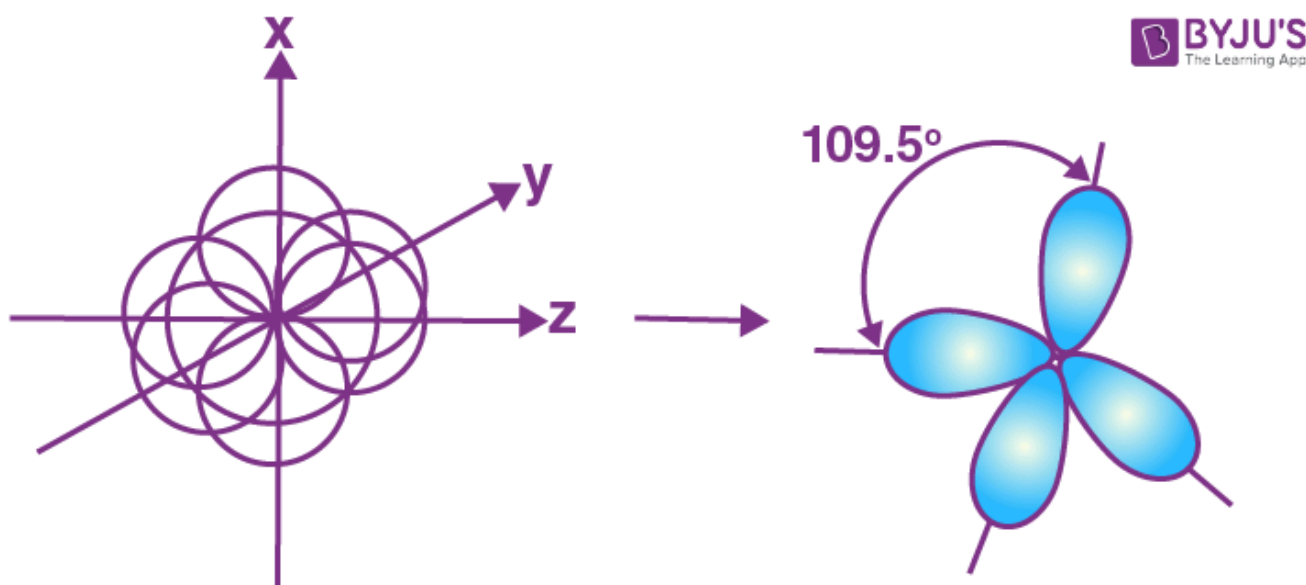
(b) sp^2 hybrid orbital

1 s- orbital hybridises with 2 p- orbitals to form 3 sp^2 hybrid orbitals. The shape of sp^2 orbital is trigonal planar.



(c) sp^3 hybrid orbital

1 s- orbital hybridises with 3 p- orbitals to form 4 sp^3 hybrid orbitals. The shape of sp^3 orbital is a tetrahedron.



Question 25

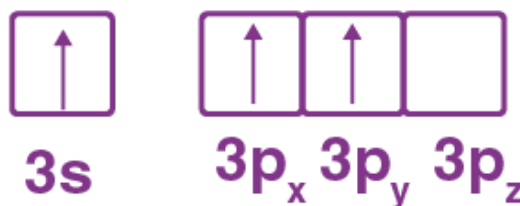
Describe the change in hybridisation (if any) of the Al atom in the following reaction.

**Solution**

The ground state of the valence orbital of Al –atom is:



In excited state the orbital picture of Al- atom is:



Thus, Al -atom in AlCl_3 undergoes sp^2 hybridisation and forms trigonal planar geometry. For the formation of



Question 26

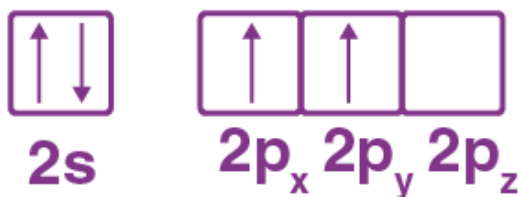
Is there any change in the hybridisation of B and N atoms as a result of the following reaction?

**Solution**

N- atom in NH_3 has sp^3 hybridization. The orbital picture of N- atom is shown below:



B- atom in BF_3 has sp^2 hybridisation . The orbital picture of B- atom is shown below:



On the reaction of NH_3 and BF_3 , $\text{F}_3\text{B} \cdot \text{NH}_3$ is obtained as a product, as hybridization of B-atom is changed to sp^3 . Although, hybridization of N- atoms remain unchanged.

Question 27

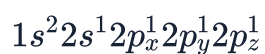
Draw diagrams showing the formation of a double bond and a triple bond between carbon atoms in C_2H_4 and C_2H_2 molecules.

Solution



The electronic configuration of a carbon atom in excited state is given below:

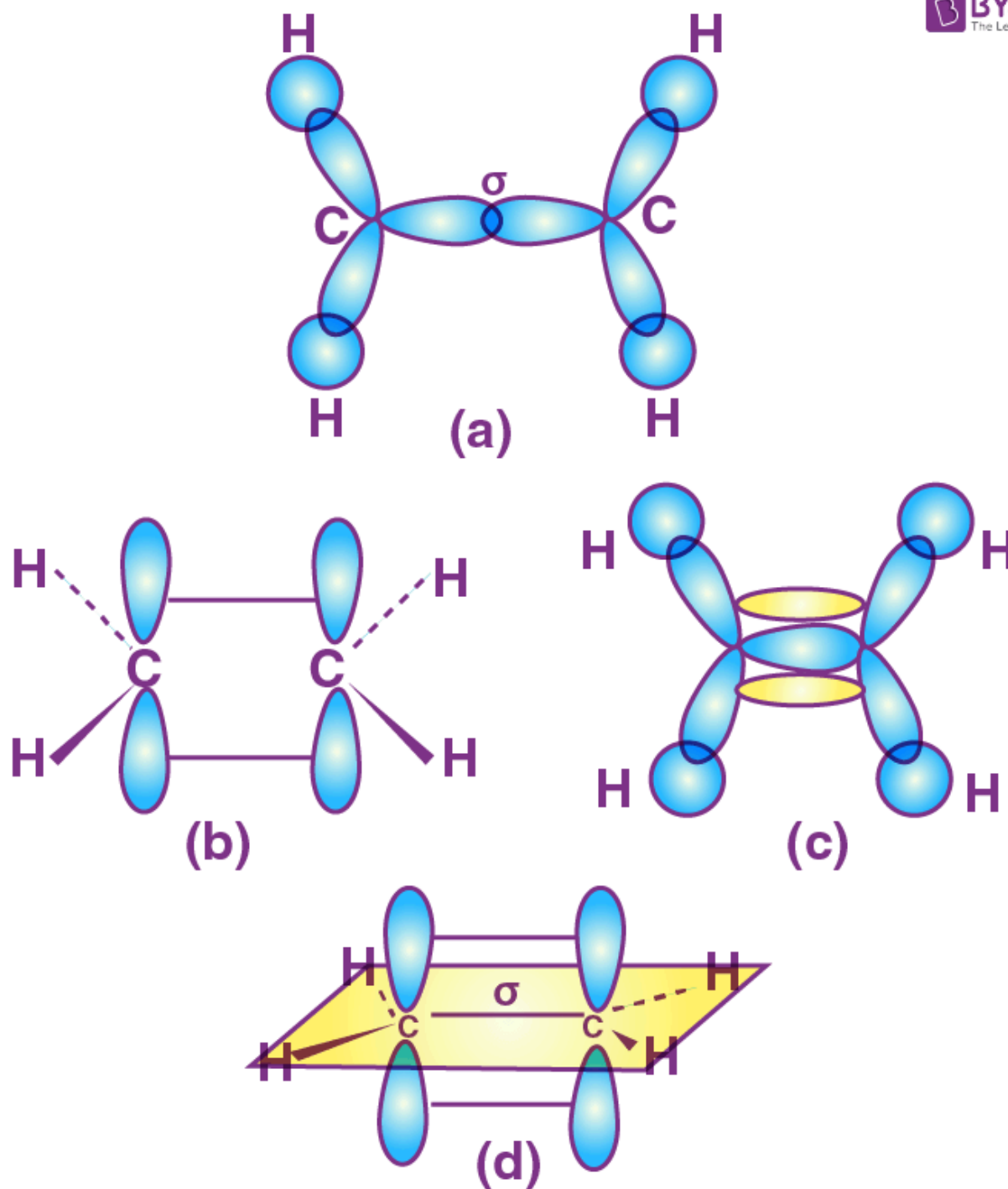
${}_6\text{C}:$



In the formation of C_2H_4 (ethane) molecule 1 sp^2 orbital of the C- atom overlaps sp^2 orbital of the other C- atom, thus forming a C-C sigma bond.

The 2 remaining sp^2 orbitals of every C- atom forms sp^2 -s

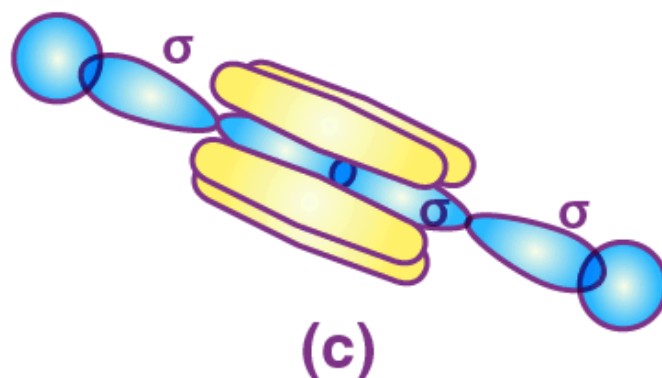
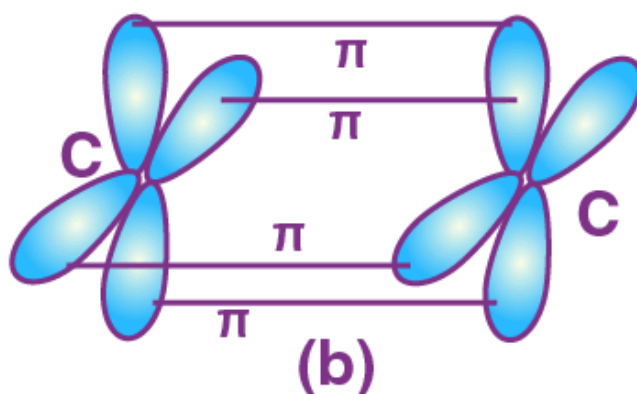
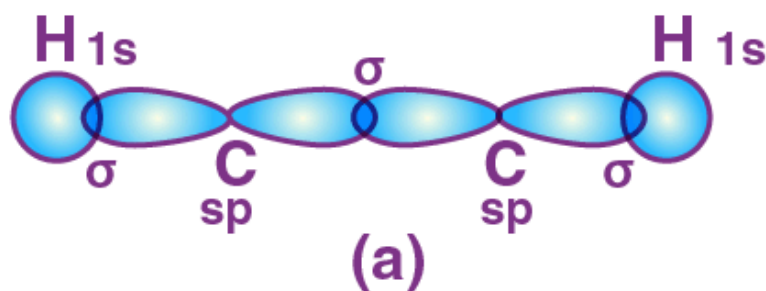
σ



In the formation of the ethyne(C_2H_2) molecule, C- atom has sp hybridization with 2 $2p$ - orbitals in an unhybridized state.

1 sp orbital of each C- atom overlaps the inter-nuclear axis and forms C-C sigma bond. The 2nd sp orbital of each C- atom overlaps half-filled 1s orbital so as to form a sigma bond.

The triple bond between the 2 C- atoms has 1 sigma bond and 2 Pie bonds. This is because 2 unhybridized 2p- orbitals overlap with the 2p- orbital of other C- atom, thus forming 2 pie bonds.



Question 28

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

(a) C_2H_2

(b) C_2H_4

Solution

A single bond is formed as the axis of bonding orbital overlaps. Thus, it forms a

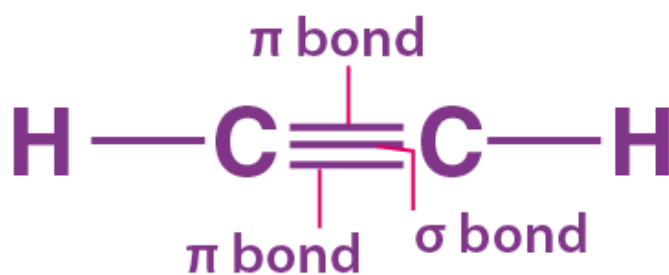
σ

π

π

σ

(a) C_2H_2



Thus, there are 2

π

σ

22

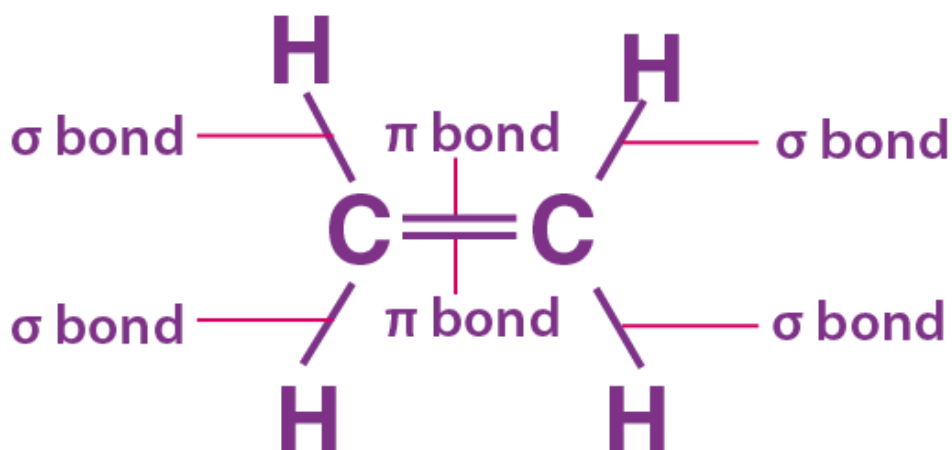
(b) C_2H_4

Thus, there are 1

π

σ

24



Question 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 $2p_x$ (c) $2p_y$ and $2p_y$ (d) $1s$ and $2s$

Solution

- (c) $2p_y$ and $2p_y$

$2p_y$ and $2p_y$ orbitals won't form a

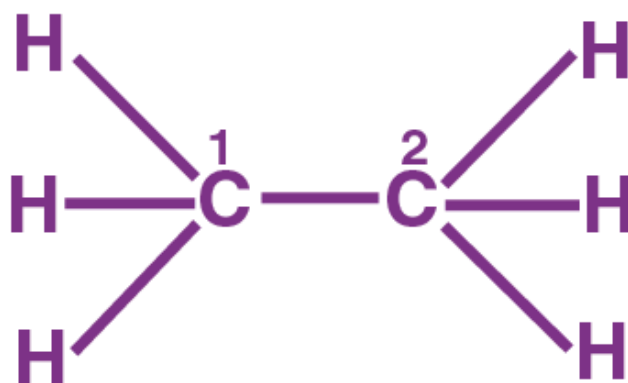
σ

π

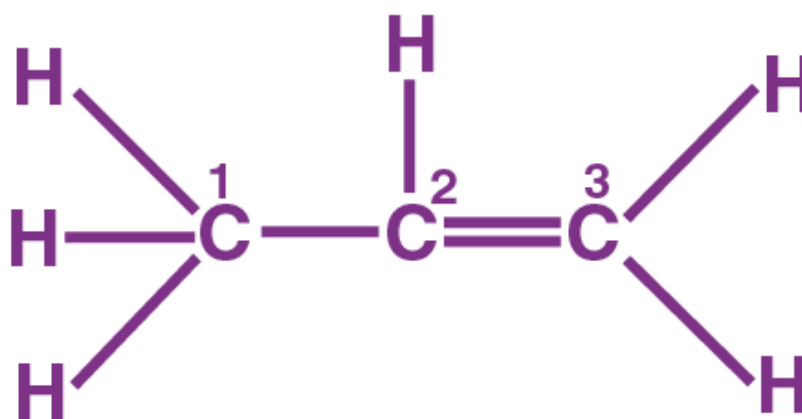
Question 30

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

- (a) $\text{CH}_3\text{-CH}_3$; (b) $\text{CH}_3\text{-CH=CH}_2$; (c) $\text{CH}_3\text{CH}_2\text{-OH}$; (d) $\text{CH}_3\text{-CHO}$; (e) CH_3COOH .

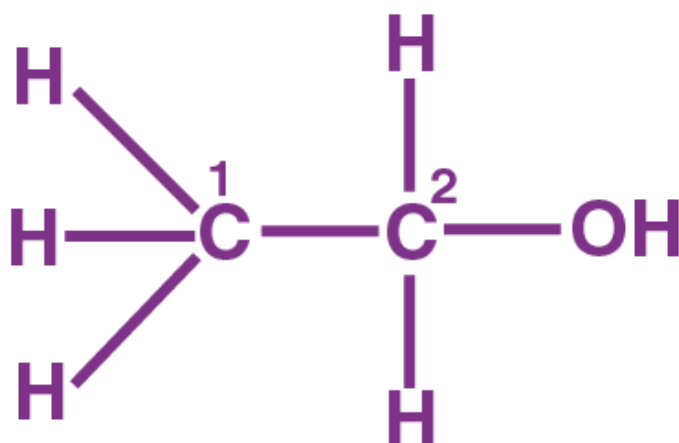
Solution(a) $\text{CH}_3\text{-CH}_3$ 

Here, C_1 and C_2 have sp^3 hybridization.

(b) $\text{CH}_3\text{-CH=CH}_2$ 

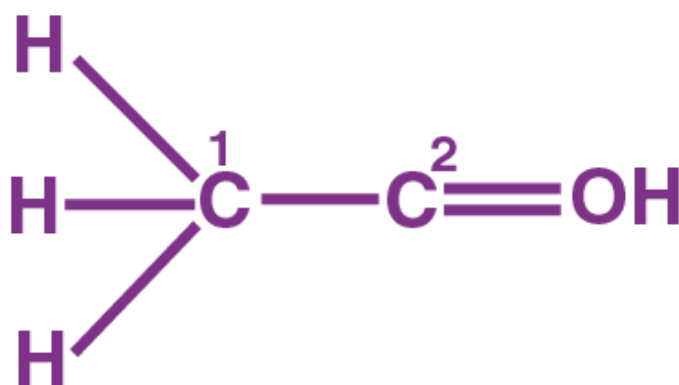
Here, C_3 and C_2 have sp^2 hybridization and C_1 has sp^3 hybridization.

(c) $\text{CH}_3\text{-CH}_2\text{-OH}$



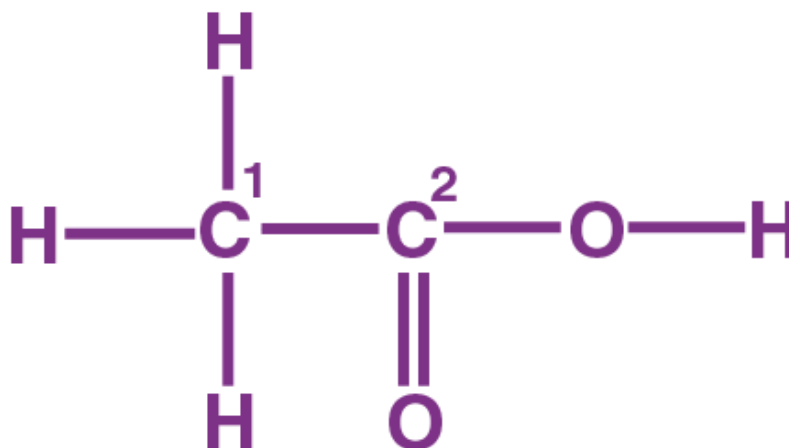
Here, C_1 and C_2 have sp^3 hybridization.

(d) CH_3-CHO



Here, C_1 has sp^3 hybridization and C_2 has sp^2 hybridization.

(e) CH_3COOH



Here, C_1 has sp^3 hybridization and C_2 has sp^2 hybridization.

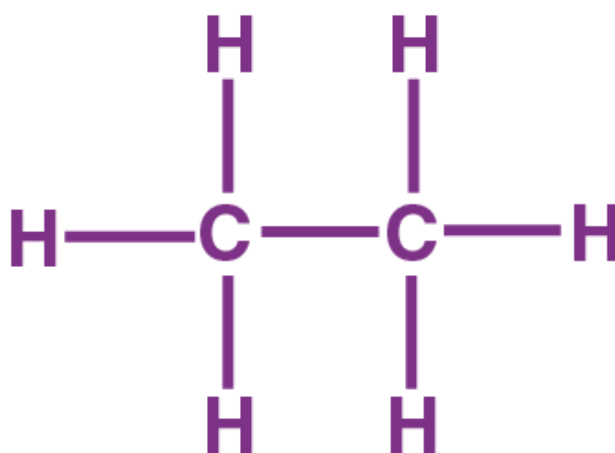
Question 31

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

Solution

A covalent bond is formed when 2 atoms combine with each other by sharing their valence electrons. The shared pairs of electrons present between the bonded atoms are called bond pairs. Each and every electron cannot participate in bonding. The pairs of electrons which do not participate in bonding are called lone pairs.

E.g. a) Ethane has 7 bond pairs but zero lone pair.



b) Water has 2 bond pairs and 2 lone pairs on O- atom.



Question 32

Distinguish between a sigma and a pi bond.

Solution

Sr. No.	Pi bond	Sigma bond
1	Pi bond is formed by lateral overlapping of orbitals.	Sigma bond is formed by end-to-end overlapping of orbitals.
2	It is a comparatively weak bond.	It is a comparatively strong bond.
3	There is only one overlapping orbital is p-p.	The overlapping orbitals are s-s, s-p, p-p.
4	Rotation around pi- bond is restricted.	Rotation is possible around sigma bond.
5	Electron cloud is not symmetrical about the line joining 2 nuclei.	Electron cloud is symmetrical about the line joining 2 nuclei.
6	It has 2 electron clouds, one above the plane of atomic nuclei and one below the plane of atomic nuclei.	It has 1 electron cloud and that is symmetrical about the inter-nuclear axis.

Question 33

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

Solution

Assuming 2 H- atoms X and Y with nuclei N_X and N_Y and electrons e_X and e_Y , respectively.

When X and Y are far from each other, there is no interaction between them. As soon as they come closer, the attractive force and repulsive force become active.

The repulsive forces are:

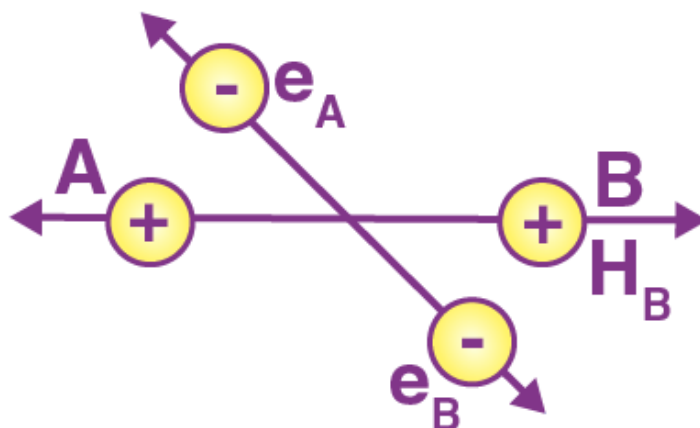
- (i) Between electrons of both the atoms, i.e., e_X and e_Y .
- (ii) Between nuclei of both the atoms, i.e., N_X and N_Y .

The attractive forces are:

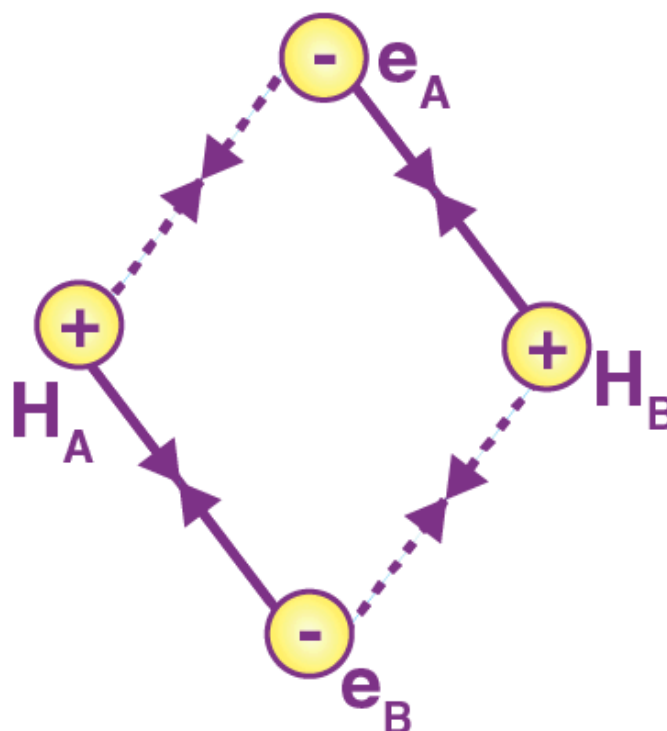
- (i) Between the electron and nucleus of the same atom i.e. $N_X - e_X$ and $N_Y - e_Y$.
- (ii) Between the electron of one atom and the nucleus of the other atom, i.e., $N_X - e_Y$ and $N_Y - e_X$.

The repulsive force pushes the 2 atoms apart, whereas the attractive force tends to bring them together.

Repulsive forces:



Attractive forces:



The values of repulsive forces are less than that of attractive forces. Thus, 2 atoms approach each other. There is a decrease in potential energy. In the end, a stage is reached when the repulsive forces balance the attractive forces, and the system achieves the minimum energy, which leads to the formation of H_2 molecule.

Question 34

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

Solution

The condition that is required for the linear combination of atomic orbitals to form molecular orbitals are as follows:

(i) The joining of atomic orbitals must have approximately the same energy. This implies in a homonuclear molecule, the 1s-orbital of one atom can join with the 1s-orbital of another atom but cannot join

with the 2s-orbital.

(ii) The joining atomic orbitals must have legitimate orientations to ensure the maximum overlap.

(iii) The overlapping must be to a large extent.

Question 35

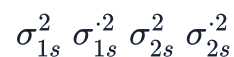
Use molecular orbital theory to explain why the Be_2 molecule does not exist.

Solution

Electronic configuration of Be:



The molecular orbital electronic configuration of Be_2 is:



Thus, bond order of Be_2 : $0.5(N_b - N_a)$.

N_b : No. of electrons in the bonding orbitals

N_a : No. of electrons in the anti-bonding orbitals

Therefore, bond order of $\text{Be}_2 = 0.5(4 - 4) = 0$

Zero value of bond order indicates that the given molecule is unstable. Thus, Be_2 doesn't exist.

Question 36

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



,
 O_2^-
(Superoxide),
 O_2^{2-}
(Peroxide)

Solution

O_2 contain 16 electrons i.e. 8 electrons from each O- atom.

- The electronic configuration of O_2 is:

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

As 1s- orbital of each O- atom does not involve in the bonding,

$$\text{No. of bonding electrons} = N_b = 8$$

$$\text{No. of anti-bonding electrons} = N_a = 4$$

Now,

$$\text{Bond order} = 0.5(8 - 4) = 2$$

- Electronic configuration of



is:

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

$$\text{No. of bonding electrons} = N_b = 8$$

$$\text{No. of anti-bonding electrons} = N_a = 3$$

Now,

$$\text{Bond order} = 0.5(8 - 3) = 2.5$$

As, bond dissociation energy

$$\propto$$

Hence, the higher the bond order, the higher stability.

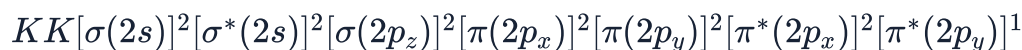
The arrangement according to decreasing order of stability is given as:



- Electronic configuration of



(Superoxide) is:



No. of bonding electrons = $N_b = 8$

No. of anti-bonding electrons = $N_a = 5$

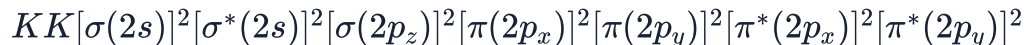
Now,

$$\text{Bond order} = 0.5(8 - 5) = 1.5$$

- Electronic configuration of



(peroxide) is:



No. of bonding electrons = $N_b = 8$

No. of anti-bonding electrons = $N_a = 6$

Now,

$$\text{Bond order} = 0.5(8 - 6) = 1$$

Question 37

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

Solution

Generally, molecular orbital is represented by the 'wave function'.

Positive (+) sign in representing a molecular orbital indicates positive wave function.

Negative (-) sign in representing a molecular orbital indicates negative wave function.

Question 38

Describe the hybridisation in case of PCl_5 . Why are the axial bonds longer as compared to equatorial bonds?

Solution

The electronic configurations of the outer orbital of phosphorus in excited state and in ground state are given below:

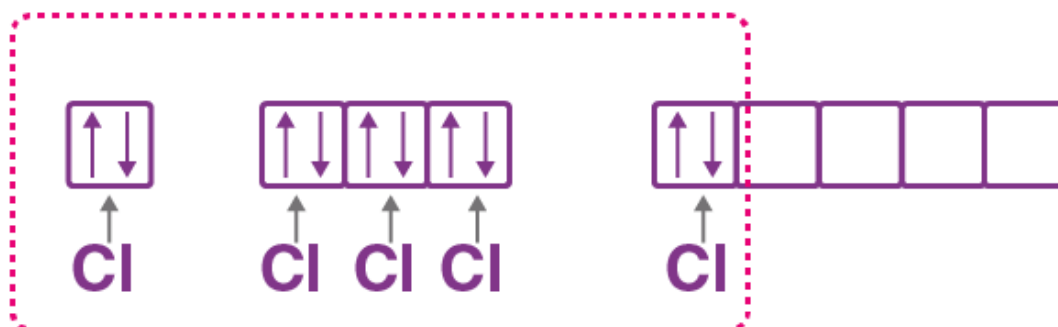
Ground State:



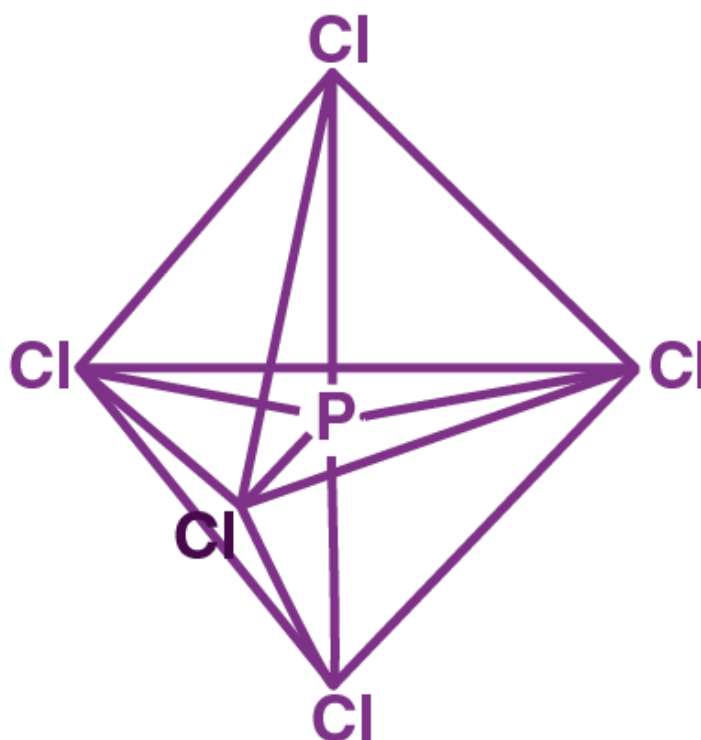
Excited State:



Phosphorus atom has sp^3d hybridization. These orbitals are filled due to the donation of electron pairs by 5 Cl^- atoms: PCl_5



The 5 sp^3d hybrid orbitals present here are directed towards 5 corners of trigonal bipyramidal. Thus, the geometry of PCl_5 is given below:



PCl_5 contains 5 P- Cl sigma bonds. Out of which, 3 P-Cl bonds lie in only 1 plane, and they are making 120°

Out of 2 remaining P-Cl bonds, one bond lie above the equatorial plane, and one bond lie below the equatorial bond. And they are making

90°

Equatorial bond pairs repel axial bond pairs to a large extent. So, equatorial bonds are slightly shorter than axial bonds.

Question 39

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

Solution

“H-bond is defined as an attractive force acting between the hydrogen attached to an electronegative atom of one molecule and an electronegative atom of a different molecule”.

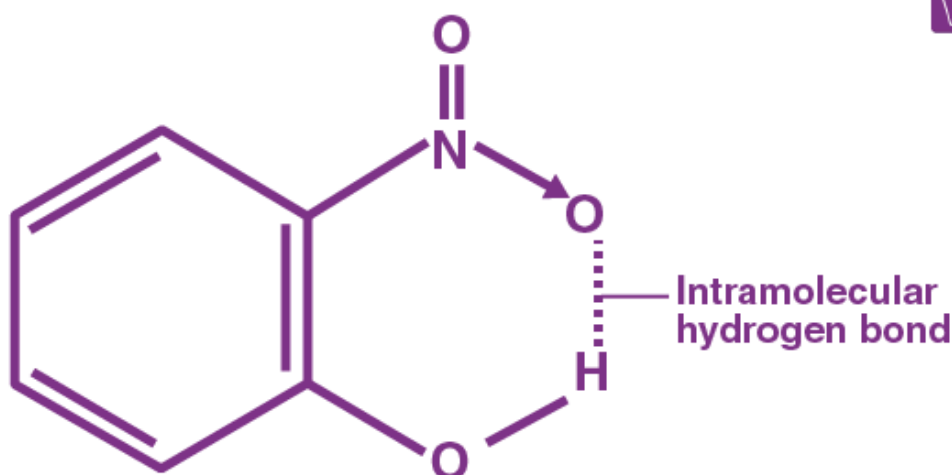
As there is a difference in the electronegativities between the atoms, the bond pair electronegative atom and hydrogen atom is drifted away from H- atom. Therefore, the hydrogen atom gets electropositive w.r.t. the other atom and procures a positive charge.



The value of H- bond is minimum in gaseous state and maximum in the solid state.

Two types of hydrogen bonds are there:

- (a) Intramolecular hydrogen bond, e.g., o- nitrophenol
- (b) Intermolecular hydrogen bond, e.g., HF, H₂O etc.



H- bonds are stronger than Van der Waals forces as H- bonds are regarded as an extreme form of the dipole-dipole interaction.

Question 40

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

Solution

Bond Order: It is defined as 0.5 times the difference between the “number of electrons present in bonding orbitals and number of electrons present in anti-bonding orbitals” of a molecule.

$$\text{Bond Order} = 0.5(N_b - N_a);$$

N_a : No. of anti-bonding electrons

N_b : No. of bonding electrons

O_2 contain 16 electrons, i.e., 8 electrons from each O- atom.

- Electronic configuration of O_2 is:

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

$$\text{No. of bonding electrons} = N_b = 8$$

$$\text{No. of anti-bonding electrons} = N_a = 4$$

Now,

$$\text{Bond order} = 0.5(8 - 4) = 2$$

- Electronic configuration of



(superoxide) is:

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

No. of bonding electrons = $N_b = 8$

No. of anti-bonding electrons = $N_a = 5$

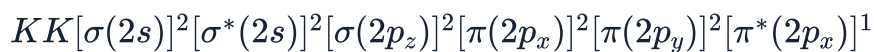
Now,

Bond order = $0.5(8 - 5) = 1.5$

- Electronic configuration of



is:



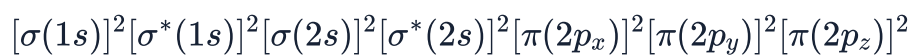
No. of bonding electrons = $N_b = 8$

No. of anti-bonding electrons = $N_a = 3$

Now,

Bond order = $0.5(8 - 3) = 2.5$

- Electronic configuration of N_2 is:



No. of bonding electrons = $N_b = 10$

No. of anti-bonding electrons = $N_a = 4$

Now,

Bond order = $0.5(10 - 4) = 3$