Chemical Bonding and Molecular Structure

1. A diatomic molecule has a dipole moment of 1.2 D, if the bond distance is 1 Å, what percentage of electronic charge exists on each atom?
2. The dipole moments of a diatomic molecule AB is 0.41D and bond distance is 2.82, calculate the % ionic character of AB.
3. The bond angle between two hybrid orbitals is 105°. Calculate the percentage of *s*-character of hybrid orbital.
4. In O_2^-, O_2 and O_2^{2-} molecular species. Find the total number of antibonding electrons.
5. There are two groups of compounds *A* and *B*. Group *A* contains three compounds Px_4, Qy_3, Rz_2. Group *B* also contains three compounds Sx_4, Ty_3, Uz_2. Hybridization of each central atom of group *A* compounds is same as that of iodine in $IBrCl^-$ while in group *B* compounds it is same as that of iodine in $IBrCl^+$. Substituents *X, Y* and *Z* exhibit covalency of one in ground state. Then find the value of *x*/*y*.

   Where, *x* and *y* are total number of lone pairs present at central atoms of compounds of group *A* and *B* respectively.
6. Consider the following three compounds (i) AX_{2n}^{n-}, (ii) AX_{3n} and (iii) AX_{4n}^{n+}, where central atom *A* is 15th group element and their maximum covalency is $3n$. If total number of proton in surrounding atom *X* is *n* and value of *n* is one, then calculate value of "$x^3 + y^2 + z$". (Where *x, y* and *z* are total number of lone pair at central atom in compound (i), (ii) and (iii) respectively.
7. Calculate the value of "$x + y - z$" here *x*, *y* and *z* are total number of non-bonded electron pair(s), pie(π) bond(s) and sigma (σ) bonds in hydrogen phosphite ion respectively.
8. Consider the following compounds:

(i) IF_5	(ii) ClI_4^-
(iii) XeO_2F_2	(iv) NH_2^-
(v) BCl_3	(vi) $BeCl_2$
(vii) $AsCl_4^+$	(viii) $B(OH)_3$
(ix) NO_2^-	(x) ClO_2^+

   The value of "$x + y - z$" is

   where *x*, *y* and *z* are total number of compounds in given compounds in which central atom used their all three p-orbitals, only two p-orbitals and only one p-orbital in hybridisation respectively.
9. Total number of species which used all three *p*-orbitals in hybridisation of central atoms and should be non-polar also are

   XeO_2F_2, $SnCl_2$, IF_5, I_3^+, XeO_4, SO_2, XeF_7^+, SeF_4
10. Consider the following orbitals $3s$, $2p_x$, $4d_{xy}$, $4d_{z^2}$, $3d_{x^2-y^2}$, $3p_y$, $4s$, $4p_z$ and find total number of orbital(s) having even number of nodal plane.
11. For the following molecules :

    PCl_5, BrF_3, ICl_2^-, XeF_5^-, NO_3^-, XeO_2F_2, PCl_4^+, CH_3^+

    Calculate the value of $\frac{a+b}{c}$

    a = Number of species having sp^3 *d*-hybridisation

    b = Number of species which are planar

    c = Number of species which are non-planar
12. Find total number of orbital which can overlap colaterally, (if inter nuclear axis is *z*) s, p_x, p_y, p_z, d_{xy}, d_{yz}, d_{xz}, d_{z^2}, $d_{x^2-y^2}$
13. The total number of lone-pairs of electrons in melamine is
14. Among the triatomic molecules/ions, $BeCl_2$, N_3^-, N_2O, NO_2^+, O_3, SCl_2, ICl_2^-, I_3^- and XeF_2, the total number of linear molecule(s)/ion(s) where the hybridization of the central atom does not have contribution from the d-orbital(s) is

    [Atomic number : S = 16, Cl = 17, I = 53 and Xe = 54]
15. The sum of the number of lone pairs of electrons on each central atom in the following species is

    $[TeBr_6]^{2-}$, $[BrF_2]^+$, SNF_3 and $[XeF_3]^-$

    (Atomic numbers: N = 7, F = 9, S = 16, Br = 35, Te = 52, Xe = 54)

SOLUTIONS

1. **(25)** $\mu = e \times d$

$$\therefore e = \frac{\mu}{d} = \frac{1.2\text{ D}}{1.0\text{ A}} = \frac{1.2 \times 10^{-18}\text{ esu cm}}{1.0 \times 10^{-8}\text{ cm}}$$

$= 1.2 \times 10^{-10}$ esu

Percentage of electronic charge

$$= \frac{1.2 \times 10^{-10}\text{ esu}}{4.8 \times 10^{-10}\text{ esu}} \times 100 = 25\%$$

2. **(76.94)** Dipole moment = electric charge × bond length

$= 4.8 \times 10^{-10} \times 2.82 \times 10^{-8} = 13.53\text{D}$

Now % ionic character

$$= \frac{\text{Actual dipole moment of the bond}}{\text{Dipole moment of pure ionic compound}} \times 100$$

then % ionic character in AB $= \frac{10.41}{13.53} \times 100 = 76.94\%$

3. **(21.44)** *s*-character $\propto$ bond angle

For 25% *s* character (as in sp^3 hybrid orbital), bond angle is 109.5°, for 33.3% *s* character (as in sp^2 hybrid orbital), bond angle is 120° and for 50% *s* character (as in *sp* hybrid orbital), bond angle is 180°.

Similarly, when the bond angle decreases below 109.5°, the *s*-character will decrease accordingly.

Decreasing in angle = 120° – 109.5° = 10.5°

Decrease in *s*-character = 33.3 – 25 = 8.3

Actual decrease in bond angle

= 109.5° – 105° = 4.5°

Expected decrease in *s*-character

$$= \frac{8.3}{10.5} \times 4.5 = 3.56\%$$

Thus, the *s*-character should decrease by about 3.56% i.e., *s*-character = 25 – 3.56 = 21.44%

4. **(21)** Molecular orbital electronic configuration of these species are :

$O_2^-(17e^-) : \sigma 1s^2, \sigma^* 1s^2, \sigma 2s^2, \sigma^* 2s^2, \sigma 2p_z^2,$

$\pi 2p_x^2 = \pi 2p_y^2, \pi^* 2p_x^2 = \pi^* 2p_y^1$

$O_2(16e^-) : \sigma 1s^2, \sigma^* 1s^2, \sigma 2s^2, \sigma^* 2s^2, \sigma 2p_z^2,$

$\pi 2p_x^2 = \pi 2p_y^2, \pi^* 2p_x^1 = \pi^* 2p_y^1$

$O_2^{2-}(18e^-) : \sigma 1s^2, \sigma^* 1s^2, \sigma 2s^2, \sigma^* 2s^2, \sigma 2p_z^2,$

$\pi 2p_x^2 : \pi 2p_y^2, \pi^* 2p_x^2 = \pi^* 2p_y^2$

Hence number of antibonding electrons are 7, 6 and 8 respectively.

5. **(2)** $I_3^- \Rightarrow sp^3d$

$[I-I-I]^-$ Hybridisation sp^3d Structure : Linear

$F-Xe-F$ Hybridisation sp^3d Structure : Linear

$N=N^+=O$ Hybridisation *sp* Structure : Linear

Group A	**l.p.**
Px_4	1
Qx_3	2
Rz_2	3

x = Total l.p. = 6

Group B	**l.p.**
Sx_4	0
Ty_3	1
Uz_2	2

Only $BeCl_2$, N_3^-, N_2O and NO_2 are linear with *sp*-hybridisation.

y = Total l.p. = 3

$x/y = 6/3 = 2$

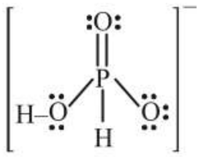
6. **(9)** $n = 1$, then $X = H$; $A = N$

(i) NH_2^- (ii) NH_3 (iii) NH_4^+

lone pair $x = 2, y = 1, z = 0$

$x^3 + y^2 + z = (2)^3 + (1)^2 + (0) = 9$

7. **(3)**



$x = 7, y = 1, z = 5$

$7 + 1 - 5 = 3$

8. **(8)** (i) $IF_5\,(sp^3d)$ (ii) $ClI_4^-\,(sp^3d^2)$

(iii) $XeO_2F_2(sp^3d)$ (iv) $NH_2^-\,(sp^3)$

(v) $BCl_3(sp^2)$ (vi) $BeCl_2\,(sp)$

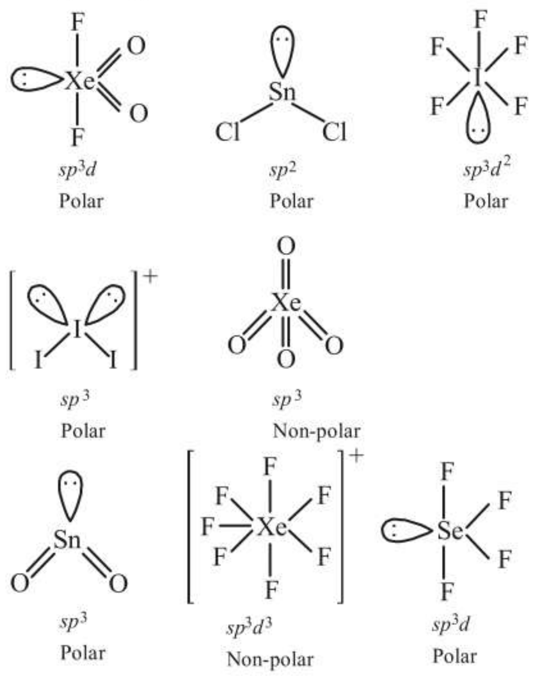
(vii) $AsCl_4^+\,(sp^3)$ (viii) $B(OH)_3\,(sp^2)$

(ix) $NO_2^-\,(sp^2)$ (x) $ClO_2^+\,(sp^2)$

$x = (sp^3)2 + sp^3d(1) + sp^3d^2(2) = 5$

$y = 4, z = 1;$ $\therefore x + y - z = 5 + 4 - 1 = 8$

9. **(2)** XeO_4, XeF_7^+



10. **(2)** $3s$: 0 Nodal plane

$4d_{z^2}$: 0 Nodal plane

$4s$: 0 Nodal plane

$2p_x$: 1 Nodal plane

$3d_{x^2-y^2}$: 2 Nodal plane

$4p_z$: 1 Nodal plane

$4d_{xy}$: 2 Nodal plane

$3p_y$: 1 Nodal plane

$4d_{xy}\ 4_{z^2}, 3d_{x^2-y^2}$, (Two)

11. **(3)** $PCl_5 \longrightarrow sp^3d$, non-planar

$BrF_3 \longrightarrow sp^3d$, bent, T-shape, planar

$ICl_2^- \longrightarrow sp^3d$, linear, planar

$XeF_5^- \longrightarrow sp^3d^3$, pentagonal planar

$NO_3^- \longrightarrow sp^2$, planar

$XeO_2F_2 \longrightarrow sp^3d$, see-saw, non-planar

$PCl_4^+ \longrightarrow sp^3$, tetrahedral, non-planar

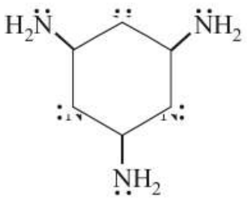
$CH_3^+ \longrightarrow sp^2$, Trigonal planar

$a = 4, b = 5, c = 3$

so, $\frac{a+b}{c} = 3$

12. **(6)** $(p_x, p_y, d_{xy}, d_{yz}, d_{xz}, d_{x^2-y^2})$

13. **(6)** Structure of melamine is as follows,

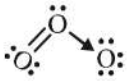


Total no. of lone pairs of electron is '6'.

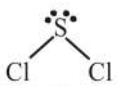
14. **(4)** $Cl-Be-Cl$
Hybridization sp
Structure : linear

$N \equiv N - \ddot{N}:^-$
Hybridisation sp
Structure : linear

$O = \overset{+}{N} \rightarrow O$
Hybridisation sp
Structure : Linear



Hybridisation sp^2
Structure : Trigonal planar



Hybridisation sp^3
Structure : Angular

$[Cl - \ddot{I} - Cl]^-$
Hybridisation sp^3d
Structure : linear

$[I - \ddot{I} - I]^-$
Hybridisation sp^3d
Structure : Linear

$F - \ddot{Xe} - F$
Hybridisation sp^3d
Structure : Linear

$\overset{-}{N} = \overset{+}{N} = O$
Hybridisation sp
Structure : Linear

Only $BeCl_2$, N_3^-, N_2O and NO_2 are linear with sp-hybridisation.

15. **(6)** Number of electron pairs around the central atom

$= \frac{V + M \pm C}{2}$

Compounds	**No. of lone pairs on central atom**
$[TeBr_6]^{2-}$	$\frac{(6+6+2)}{2} - 6 = 1$
$[BrF_2]^+$	$\frac{(7+2-1)}{2} - 2 = 2$
SNF_3	$\frac{6-1+3}{2} - 4 = 0$
$[XeF_3]^-$	$\frac{(8+3+1)}{2} - 3 = 3$

$\therefore$ Sum of number of lone pairs $= 1 + 2 + 0 + 3 = 6$