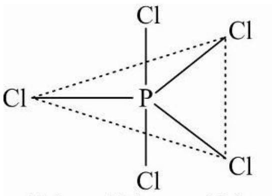
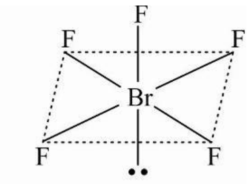
76. ***Pcl***$_5$ **→ triangular bipyramidal, BrF$_5$ → square pyramidal**

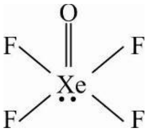


Trigonal bipyramidal
(P is sp^3d-hybridised)



Square pyramidal
(Br is sp^3d^2-hybridised)

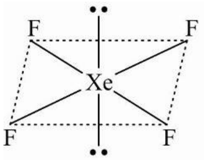
77.(C) At central atom (Xe), there is one lone pair and each F has three lone pairs while O has two lone pairs.



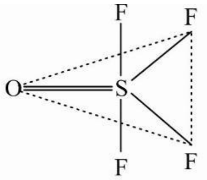
78. $\boldsymbol{O_2^+ < O_2 < O_2^-}$

Bond order : $O_2^- = 1.5, O_2 = 2, O_2^{2+} = 2.5$. Bond length : $O_2^+ < O_2 < O_2^-$

79. ***XeF***$_4$ **→ square planar**
OsF$_4$ → triangular bipyramidal



Square planar



Trigonal bipyramidal

80.(A) $O_2^+(15e^-) : \sigma 1s^2\, \overset{*}{\sigma}1s^2\, \sigma 2s^2\, \overset{*}{\sigma}2s^2 \sigma 2p_x^2 \left|\begin{matrix}\pi 2p_y^2 \\ \pi 2p_z^2\end{matrix}\right|\begin{matrix}\overset{*}{\pi}2p_y^1 \\ \overset{*}{\pi}2p_z^0\end{matrix}\Bigg|\, \overset{*}{\sigma}2p_x^0$

Bond order $= \dfrac{10-5}{2} = 2.5$; paramagnetic.

$O_2(16e^-) : \sigma 1s^2\, \overset{*}{\sigma}1s^2\, \sigma 2s^2\, \overset{*}{\sigma}2s^2 \sigma 2p_x^2 \left|\begin{matrix}\pi 2p_y^2 \\ \pi 2p_z^2\end{matrix}\right|\begin{matrix}\overset{*}{\pi}2p_y^1 \\ \overset{*}{\pi}2p_z^1\end{matrix}\Bigg|\, \overset{*}{\sigma}2p_x$

Bond order $= \dfrac{10-6}{2} = 2$. Hence, (A) is the correct answer.

81. **NO**

No, (i) NMe_3 is pyramidal while (ii) $N(SiMe_3)_3$ is planar. In the latter case, $p\pi - d\pi$ back bonding between N and Si makes N sp^2 – hybridised.

82.(D) I_3^- : No. of $\ell p = 3$

83.(D) O_2^- in KO_2 has 17 electrons, species with odd electrons are always paramagnetic.

84.(A) The bond order of CO = 3. NO^+, CN^- and N_2 are isoelectronic with CO, have the same bond order as CO. NO^- $(16e^-)$ has bond order of 2.

85. A → p, q, r, t; B → q, r, s, t; C → p, q, r; A → p, q, r, s

(A) $B_2 : \sigma 1s^2 \overset{*}{\sigma} 1s^2 \sigma 2s^2 \overset{*}{\sigma} 2s^2 \left| \begin{matrix} \pi 2p_y^1 \\ \pi 2p_z^1 \end{matrix} \right|$ paramagnetic. Bond order $= \dfrac{6-4}{2} = 1$

Bond is formed by mixing of s and p orbitals. B_2 undergoes both oxidation & reduction as

$B_2 + O_2 \xrightarrow{\text{Heat}} B_2O_3$ (Oxidation)

$B_2 + H_2 \longrightarrow B_2H_6$ (Reduction)

(B) $N_2 : \sigma 1s^2 \overset{*}{\sigma} 1s^2 \sigma 2s^2 \overset{*}{\sigma} 2s^2 \sigma 2p_x^2 \left| \begin{matrix} \pi 2p_y^2 \\ \pi 2p_z^2 \end{matrix} \right|$ diamagnetic. Bond order $= \dfrac{10-4}{2} = 3 > 2$

N_2 undergoes both oxidation and reduction as

$N_2 + O_2 \xrightarrow{\Delta} NO$; $N_2 + 3H_2 \xrightarrow{\text{Catalyst}} NH_3$

In N_2, bonds are formed by mixing of s and p orbitals.

(C) $O_2^- : \sigma 1s^2 \overset{*}{\sigma} 1s^2 \sigma 2s^2 \overset{*}{\sigma} 2s^2 \sigma 2p_x^2 \left| \begin{matrix} \pi 2p_y^2 \\ \pi 2p_z^2 \end{matrix} \right| \left| \begin{matrix} \overset{*}{\pi} 2p_y^2 \\ \overset{*}{\pi} 2p_z^1 \end{matrix} \right| \overset{*}{\sigma} 2p_x^0$

Paramagnetic with bond order $= 1.5. O_2^-$ undergoes both oxidation and reduction

(D) $O_2 : \sigma 1s^2 \overset{*}{\sigma} 1s^2 \sigma 2s^2 \overset{*}{\sigma} 2s^2 \sigma 2p_x^2 \left| \begin{matrix} \pi 2p_y^2 \\ \pi 2p_z^2 \end{matrix} \right| \left| \begin{matrix} \overset{*}{\pi} 2p_y^1 \\ \overset{*}{\pi} 2p_z^1 \end{matrix} \right| \overset{*}{\sigma} 2p_x^0$

Paramagnetic with bond order = 2. O_2 undergoes reduction and oxidation

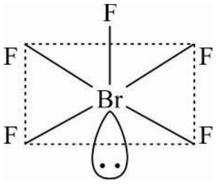
86.(A) For molecules lighter than O_2, the increasing order of energies of molecular orbitals is

$$\sigma 1s \overset{*}{\sigma} 1s \sigma 2s \overset{*}{\sigma} 2s \begin{bmatrix} \pi 2p_y \\ \pi 2p_z \end{bmatrix} \sigma 2p_x \begin{bmatrix} \overset{*}{\pi} 2p_y \\ \overset{*}{\pi} 2p_z \end{bmatrix} \overset{*}{\sigma} 2p_x$$

where, $\pi 2p_y$ and $\pi 2p_z$ are degenerate molecular orbitals, first singly occupied and then pairing starts if Hund's rule is obeyed. If Hund's rule is violated in C_2, electronic arrangement would not change and no change in bond order and magnetic property.

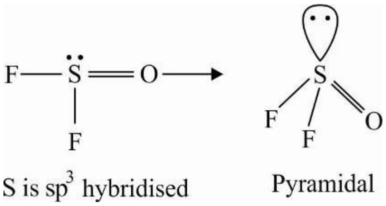
$$\sigma 1s^2 \overset{*}{\sigma} 1s^2 \sigma 2s^2 \overset{*}{\sigma} 2s^2 \left[\begin{matrix} \pi 2p_y^2 ..... \\ \pi 2p_z \end{matrix} \right.$$

87.(0)



Lone pair would push the Br–F bond pairs in upward direction and all Br^-F bond angles will contract.

88.(D) SO_3 is planar (S is sp^2 hybridised), BrF_3 is T-shaped and SiO_3^{2-} is planar (Si is sp^2 hybridised).



89.(AB) $C_2(6+6=12) = \sigma 1s^2, \overset{*}{\sigma}\ 1s^2, \sigma 2s^2, \overset{*}{\sigma}\ 2s^2, \pi 2p_y^2$

Since, all the electrons are paired, it is a diamagnetic species.

$N_2(7+7=14) = \sigma 1s^2, \overset{*}{\sigma}1s^2, \sigma 2s^2, \overset{*}{\sigma}\ 2s^2, \pi 2p_x^2 = \pi 2p_y^2, \sigma 2p_z^2$

It is also a diamagnetic species because of the absence of unpaired electrons.

$O_2\,(8+8=16)$

or $S_2 = \sigma 1s^2, \overset{*}{\sigma}1s^2, \sigma 2s^2, \overset{*}{\sigma}\ 2s^2, \sigma 2s_z^2, \pi 2p_x^2 = \pi 2p_y^2, \overset{*}{\pi}2p_x^1 = \overset{*}{\pi}2p_y^1$

Due to the presence of two unapired electrons, O_2 and S_2 both are paramagnetic molecules.

90.(C) This problem can be solved by using the concept involved in molecular orbital theory. Write the molecular orbital electronic configuration keeping in mind that there is no 2s-2p mixing, then if highest occupied molecular orbital contain unpaired electron then molecule is paramagnetic otherwise diamagnetic.

Assuming that no 2s-2p mixing takes place the molecular orbital electronic configuration can be written in the following sequence of $\sigma 1s, \overset{*}{\sigma}1s, \sigma 2s\ \overset{*}{\sigma}2s, \sigma 2p_z, \pi 2p_x \equiv \pi 2p_y, \overset{*}{\pi}2p_x \equiv \overset{*}{\pi}2p_y, \overset{*}{\sigma}2p_z$

(a) $Be_2 \rightarrow \sigma 1s^2, \overset{*}{\sigma}1s^2, \sigma 2s^2\ \overset{*}{\sigma}2s^2$ (diamagnetic)

(b) $B_2 \rightarrow \sigma 1s^2, \overset{*}{\sigma}1s^2, \sigma 2s^2, \overset{*}{\sigma}2s^2, \overset{*}{\sigma}2p_z^2, \begin{matrix}\pi 2p_x^0\\ \pi 2p_y^0\end{matrix}$ (diamagnetic)

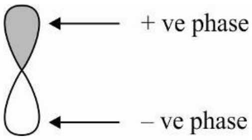
(c) $C_2 \rightarrow \sigma 1s^2, \overset{*}{\sigma}1s^2, \sigma 2s^2, \overset{*}{\sigma}2s^2, \overset{*}{\sigma}2p_z^2, \begin{matrix}\pi 2p_x^1\\ \pi 2p_y^1\end{matrix}, \overset{*}{\pi}2p_x^0, \overset{*}{\sigma}2p_z^0$ (diamagnetic)

(d) $N_2 \rightarrow \sigma 1s^2, \overset{*}{\sigma}1s^2, \sigma 2s^2, \overset{*}{\sigma}2s^2, \overset{*}{\sigma}2p_z^2, \begin{matrix}\pi 2p_x^2\\ \pi 2p_y^2\end{matrix}, \begin{matrix}\overset{*}{\pi}2p_x^0\\ \overset{*}{\pi}2p_y^2\end{matrix}, \sigma * 2p_z^0$ (diamagnetic)

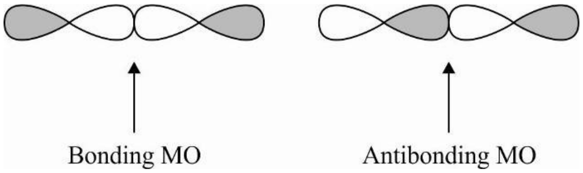
Hence, (C) is the correct choice.

91.(ABD) This problem can be solved by using concept of H-bonding and applications of H-bonding.

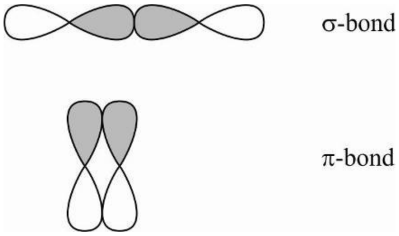
92.(C) This problem includes basic concept of bonding. It can be solved by using the concept of molecular orbital theory



Any orbitals has two phase +ve and –ve. In the following diagram, +ve phase is shown by darkening the lobes and –ve by without darkening the lobes.

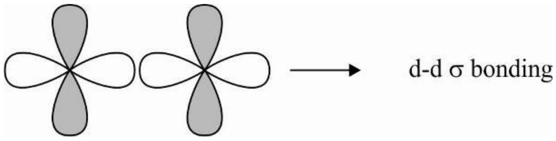


When two same phase overlap with each other, it forms bonding molecular orbital otherwise antibonding.

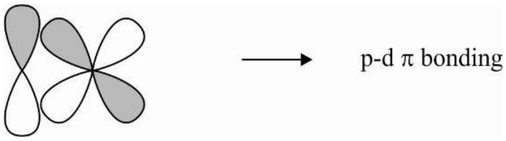


On the basis of above two concepts, correct matching can be done as shown below:

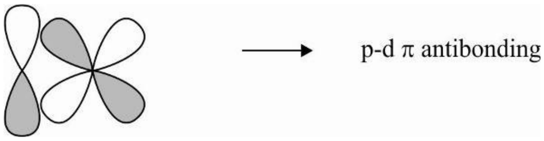
[p]



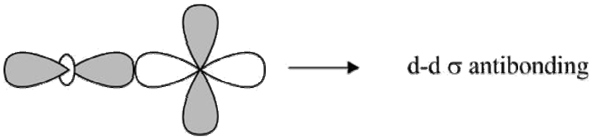
[q]



[r]



[s]



Hence, (C) is the correct option.

93.(4) $BeCl_2, N_3^-, N_2O, NO_2^+$

94.(BC) $BrF_5 = 1\ell p$, $XeF_4 = 2\ell p$; $C\ell F_3 = 2\ell p$, $SF_4 = 1\ell p$

95.(AC)

Species	**Electrons**	**MOEC**	**N_B**	**N_A**	**BO**	**Magnetic character**
C_2^{2-}	14	$\sigma 1s^2, \sigma^* 1s^2, \sigma 2s^2, \sigma^* 2s^2,$ $\pi 2p_x^2 \approx -\pi 2p_y^2, \sigma 2p_z^2$	10	4	3	Diamagnetic

O_2^{2+}	14	As above according to number of electrons	10	4	3	Diamagnetic
O_2	16		10	6	2	Paramagnetic
N_2^+	13		9	4	2.5	Paramagnetic
N_2^-	15		10	5	2.5	Paramagnetic
He_2^+	3		2	1	0.5	Paramagnetic

Thus, (a) is correct.

(b) Bond order $O_2^{2+} > O_2$ thus, Both length of $O_2^{2+} < O_2$ thus, incorrect.

(c) N_2^+ and N_2^- have same bond order thus correct.

(d) He_2^+ with bond order = 0.5 is more stable thus, less energy than isolated He atoms. Thus, (d) incorrect.

96.(6)

	Number of ℓp		Number of ℓp
$TeBr_6^{2-}$	1	BrF_2^+	2
SNF_3	0	XeF_3^-	3

Total $\ell p = 6$

97.(5) H_2, Li_2, C_2, N_2, F_2

98.(CD) **(C)** NO_2, NH_3, $POCl_3$, CH_3Cl (polar molecule)

(D) SO_2, C_6H_5Cl, H_2Se, BrF_5 (polar molecule)