4

Chemical Bonding and Molecular Structure

TOPIC 1 Electrovalent, Covalent and Co-ordinate Bonding

1. Which of the following compounds contain(s) no covalent bond(s)? KCl, PH_3, O_2, B_2H_6, H_2SO_4 **[2018]**

(a) KCl, B_2H_6, PH_3 (b) KCl, H_2SO_4

(c) KCl (d) KCl, B_2H_6

2. Amongst LiCl, RbCl, $BeCl_2$ and $MgCl_2$ the compounds with the greatest and the least ionic character, respectively are: **[Online April 19, 2014]**

(a) LiCl and RbCl (b) RbCl and $BeCl_2$

(c) $MgCl_2$ and $BeCl_2$ (d) RbCl and $MgCl_2$

3. Which of these statements is not true? **[Online April 19, 2014]**

(a) NO^+ is not isoelectronic with O_2

(b) B is always covalent in its compounds

(c) In aqueous solution, the Tl^+ ion is much more stable than Tl (III)

(d) $LiAlH_4$ is a versatile reducing agent in organic synthesis.

4. Lattice energy of an ionic compound depends upon

(a) Charge on the ion and size of the ion **[2005]**

(b) Packing of ions only

(c) Size of the ion only

(d) Charge on the ion only

TOPIC 2 Octet rule, Resonance and Hydrogen Bonding

5. *ortho*-Nitrophenol is less soluble in water than *p*- and *m*- nitrophenols because : **[2012]**

(a) *o*-nitrophenol is more volatile steam than those of *m*- and *p*-isomers.

(b) *o*-nitrophenol shows intramolecular H-bonding

(c) *o*-nitrophenol shows intermolecular H-bonding

(d) Melting point of *o*-nitrophenol is lower than those of *m*- and *p*-isomers.

6. Among the following, the species having the smallest bond length is **[Online May 7, 2012]**

(a) NO^- (b) NO^+ (c) O_2 (d) NO

7. Which one of the following pairs of species have the same bond order? **[2008]**

(a) CN^- and NO^+ (b) CN^- and CN^+

(c) O^-_2 and CN^- (d) NO^+ and CN^+

8. Which of the following hydrogen bonds is strongest?

(a) O – H - - - F (b) O – H - - - H **[2007]**

(c) F – H - - - F (d) O – H - - - O.

9. The bond order in NO is 2.5 while that in NO^+ is 3. Which of the following statements is true for these two species ?

(a) Bond length in NO^+ is equal to that in NO **[2004]**

(b) Bond length in NO is greater than in NO^+

(c) Bond length in NO^+ is greater than in NO

(d) Bond length is unpredictable

10. An ether is more volatile than an alcohol having the same molecular formula. This is due to **[2003]**

(a) alcohols having resonance structures

(b) intermolecular hydrogen bonding in ethers

(c) intermolecular hydrogen bonding in alcohols

(d) dipolar character of ethers

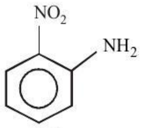
TOPIC 3 Dipole Moment and Bond Polarity

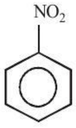
11. The dipole moments of CCl_4, $CHCl_3$ and CH_4 are in the order: **[Jan. 07, 2020 (I)]**

(a) $CHCl_3 < CH_4 = CCl_4$ (b) $CCl_4 < CH_4 < CHCl_3$

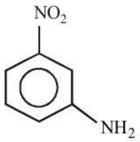
(c) $CH_4 < CCl_4 < CHCl_3$ (d) $CH_4 = CCl_4 < CHCl_3$

12. Which compound exhibits maximum dipole moment among the following ? **[Online April 11, 2015]**

(a)


(b)


(c)


(d)


13. Molecule AB has a bond length of 1.617Å and a dipole moment of 0.38 D. The fractional charge on each atom (absolute magnitude) is : ($e_0 = 4.802 \times 10^{-10}$ esu) **[Online April 11, 2015]**

(a) 0.5 (b) 0.05 (c) 0 (d) 1.0

14. The correct order of bond dissociation energy among N_2, O_2, O_2^- is shown in which of the following arrangements? **[Online April 11, 2014]**

(a) $N_2 > O_2^- > O_2$ (b) $O_2^- > O_2 > N_2$

(c) $N_2 > O_2 > O_2^-$ (d) $O_2 > O_2^- > N_2$

15. Which one of the following molecules is polar ? **[Online April 9, 2013]**

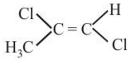
(a) XeF_4 (b) IF_5 (c) SbF_5 (d) CF_4

16. Bond distance in HF is 9.17×10^{-11} m. Dipole moment of HF is 6.104×10^{-30} Cm. The percentage ionic character in HF will be : (electron charge $= 1.60 \times 10^{-19}$ C) **[Online April 23, 2013]**

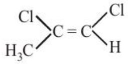
(a) 61.0% (b) 38.0% (c) 35.5% (d) 41.5%

17. Among the following chloro-compound having the lowest dipole moment is **[Online May 12, 2012]**

(a) CH_3Cl

(b) 

(c) CH_2Cl_2

(d) 

18. Although CN^- ion and N_2 molecule are isoelectronic, yet N_2 molecule is chemically inert because of **[Online May 12, 2012]**

(a) presence of more number of electrons in bonding orbitals
(b) low bond energy
(c) absence of bond polarity
(d) uneven electron distribution.

19. The charge/size ratio of a cation determines its polarizing power. Which one of the following sequences represents the increasing order of the polarizing power of the cationic species, K^+, Ca^{2+}, Mg^{2+}, Be^{2+}? **[2007]**

(a) $Ca^{2+} < Mg^{2+} < Be^+ < K^+$
(b) $Mg^{2+} < Be^{2+} < K^+ < Ca^{2+}$
(c) $Be^{2+} < K^+ < Ca^{2+} < Mg^{2+}$
(d) $K^+ < Ca^{2+} < Mg^{2+} < Be^{2+}$.

20. Which one of the following pairs of molecules will have permanent dipole moments for both members ? **[2003]**

(a) NO_2 and CO_2 (b) NO_2 and O_3

(c) SiF_4 and CO_2 (d) SiF_4 and NO_2

TOPIC 4 VSEPR Theory and Hybridisation

21. The compound that has the largest H – M – H bond angle (M = N, S, C), is : **[Sep. 05, 2020 (II)]**

(a) H_2O (b) NH_3

(c) H_2S (d) CH_4

22. The molecule in which hybrid MOs involve only one *d*-orbital of the central atom is : **[Sep. 04, 2020 (II)]**

(a) $[Ni(CN)_4]^{2-}$ (b) BrF_5

(c) XeF_4 (d) $[CrF_6]^{3-}$

23. If AB_4 molecule is a polar molecule, a possible geometry of AB_4 is : **[Sep. 02, 2020 (I)]**

(a) Square pyramidal (b) Tetrahedral

(c) Rectangular planar (d) Square planar

24. The shape/ structure of $[XeF_5]^-$ and XeO_3F_2, respectively, are : **[Sep. 02, 2020 (II)]**

(a) pentagonal planar and trigonal bipyramidal
(b) octahedral and square pyramidal
(c) trigonal bipyramidal and pentagonal planar
(d) trigonal bipyramidal and trigonal bipyramidal

25. The molecular geometry of SF_6 is octahedral. What is the geometry of SF_4 (including lone pair(s) of electrons, if any)? **[Sep. 02, 2020 (II)]**

(a) Tetrahedral (b) Trigonal bipyramidal

(c) Pyramidal (d) Square planar

26. The correct statement about ICl_5 and ICl_4^- is : **[April 8, 2019 (II)]**

(a) both are is isostructural.
(b) ICl_5 is trigonal bipyramidal and ICl_4^- is tetrahedral.
(c) ICl_5 is square pyramidal and ICl_4^- is tetrahedral.
(d) ICl_5 is square pyramidal and ICl_4^- is square planar.

27. The ion that has sp^3d^2 hydridisation for the central atom, is: **[April 8, 2019 (II)]**

(a) $[ICl_4]^-$ (b) $[ICl_2]^-$ (c) $[IF_6]^-$ (d) $[BrF_2]^-$

28. Total number of lone pair of electrons in I_3^- ion is :**[2018]**

(a) 3 (a) 6 (c) 9 (d) 12

29. Which of the following conversions involves change in both shape and hybridisation? **[Online April 16, 2018]**

(a) $H_2O \rightarrow H_3O^+$ (b) $BF_3 \rightarrow BF_4^-$

(c) $CH_4 \rightarrow C_2H_6$ (d) $NH_3 \rightarrow NH_4^+$

30. The incorrect geometry is represented by __________. **[Online April 16, 2018]**

(a) NF_3- trigonal planar
(b) BF_3- trigonal planar
(c) AsF_5- trigonal bipyramidal
(d) H_2O- bent

31. Identify the pair in which the geometry of the species is T-shape and square pyramidal, respectively **[Online April 15, 2018 (I)]**

(a) ICl_2^- and ICl_5 (b) IO_3^- and $IO_2F_2^-$

(c) ClF_3 and IO_4^- (d) $XeOF_2$ and $XeOF_4$

32. The decreasing order of bond angles in BF_3, NH_3, PF_3 and I_3^- is : **[Online April 15, 2018 (I)]**

(a) $I_3^- > BF_3 > NH_3 > PF_3$ (b) $BF_3 > I_3^- > PF_3 > NH_3$

(c) $BF_3 > NH_3 > PF_3 > I_3^-$ (d) $I_3^- > NH_3 > PF_3 > BF_3$

33. sp^3d^2 Hybridisation is not displayed by : **[Online April 8, 2017]**
(a) BrF_5 (b) SF_6
(c) $[CrF_6]^{3-}$ (d) PF_5

34. The group having triangular planar structures is : **[Online April 9, 2017]**
(a) BF_3, NF_3, CO_3^{2-} (b) CO_3^{2-}, NO_3^-, SO_3
(c) NH_3, SO_3, CO_3^{2-} (d) NCl_3, BCl_3, SO_3

35. The species in which the N atom is in a state of *sp* hybridisation is : **[2016]**
(a) NO_3^- (b) NO_2 (c) NO_2^+ (d) NO_2^-

36. The group of molecules having identical shape is : **[Online April 9, 2016]**
(a) PCl_5, IF_5, XeO_2F_2 (b) BF_3, PCl_3, XeO_3
(c) SF_4, XeF_4, CCl_4 (d) $ClF_3, XeOF_2, XeF_3^+$

37. The bond angle H–X–H is the greatest in the compound : **[Online April 10, 2016]**
(a) PH_3 (b) CH_4 (c) NH_3 (d) H_2O

38. The number and type of bonds in C_2^{2-} ion in CaC_2 are:
(a) One σ bond and one π-bond **[Online April 9, 2014]**
(b) One σ bond and two π-bond
(c) Two σ bond and two π-bond
(d) Two σ bond and one π-bond

39. Which of the following molecules has two sigma (σ) and two pi (π) bonds? **[Online April 12, 2014]**
(a) C_2H_4 (b) N_2F_2 (c) $C_2H_2Cl_2$ (d) HCN

40. The shape of IF_6^- is : **[Online April 23, 2013]**
(a) Trigonally distorted octahedron
(b) Pyramidal
(c) Octahedral
(d) Square antiprism

41. In which of the following sets, all the given species are isostructural ? **[Online April 25, 2013]**
(a) CO_2, NO_2, ClO_2, SiO_2 (b) $PCl_3, AlCl_3, BCl_3, SbCl_3$
(c) BF_3, NF_3, PF_3, AlF_3 (d) $BF_4^-, CCl_4, NH_4^+, PCl_4^+$

42. In which of the following pairs, the two species are not isostructural ? **[2012]**
(a) CO_3^{2-} and NO_3^- (b) PCl_4^+ and $SiCl_4$
(c) PF_5 and BrF_5 (d) AlF_6^{3-} and SF_6

43. The formation of molecular complex BF_3-NH_3 results in a change in hybridisation of boron **[Online May 12, 2012]**
(a) from sp^2 to dsp^2 (b) from sp^2 to sp^3
(c) from sp^3 to sp^2 (d) from sp^3 to sp^3d

44. Which of the following has the square planar structure? **[Online May 19, 2012]**
(a) XeF_4 (b) NH_4^+ (c) BF_4^- (d) CCl_4

45. Among the following species which two have trigonal bipyramidal shape? **[Online May 26, 2012]**
(I) NI_3 (II) I_3^- (III) SO_3^{2-} (IV) NO_3^-
(a) I and III (b) III and IV (c) I and IV (d) II and III

46. The bond dissociation energy of B – F in BF_3 is 646 kJ mol^{-1}, whereas that of C – F in CF_4 is 515 kJ mol^{-1}. The correct reason for higher B – F bond dissociation energy as compared to that of C – F bond is **[2008]**
(a) stronger σ bond between B and F in BF_3 as compared to that between C and F in CF_4.
(b) significant $p\pi - p\pi$ interaction between B and F in BF_3, whereas there is no possibility of such interaction between C and F in CF_4.
(c) lower degree of $p\pi - p\pi$ interaction between B and F in BF_3 than that between C and F in CF_4.
(d) smaller size of B– atom as compared to that of C– atom.

47. In which of the following molecules/ions are all the bonds **not** equal? **[2006]**
(a) XeF_4 (b) BF_4^- (c) SF_4 (d) SiF_4

48. The decreasing values of bond angles from NH_3 (106°) to SbH_3 (101°) down group-15 of the periodic table is due to
(a) decreasing *lp-bp* repulsion **[2006]**
(b) decreasing electronegativity
(c) increasing *bp-bp* repulsion
(d) increasing *p*-orbital character in sp^3

49. The correct order of bond angles (smallest first) in H_2S, NH_3, BF_3 and SiH_4 is **[2004]**
(a) $H_2S < NH_3 < SiH_4 < BF_3$
(b) $NH_3 < H_2S < SiH_4 < BF_3$
(c) $H_2S < SiH_4 < NH_3 < BF_3$
(d) $H_2S < NH_3 < BF_3 < SiH_4$

50. The states of hybridization of boron and oxygen atoms in boric acid (H_3BO_3) are respectively **[2004]**
(a) sp^3 and sp^2 (b) sp^2 and sp^3
(c) sp^2 and sp^2 (d) sp^3 and sp^3

51. Which one of the following has the regular tetrahedral structure ? **[2004]**
(a) BF_4^- (b) SF_4
(c) XeF_4 (d) $[Ni(CN)_4]^{2-}$
(Atomic nos. : B = 5, S = 16, Ni = 28, Xe = 54)

52. The maximum number of 90° angles between bond pair-bond pair of electrons is observed in **[2004]**
(a) dsp^2 hybridization (b) sp^3d hybridization
(c) dsp^3 hybridization (d) sp^3d^2 hybridization

53. Which one of the following compounds has the smallest bond angle in its molecule ? **[2003]**
(a) OH_2 (b) SH_2 (c) NH_3 (d) SO_2

54. The pair of species having identical shapes for molecules of both species is **[2003]**
(a) XeF_2, CO_2 (b) BF_3, PCl_3
(c) PF_5, IF_5 (d) CF_4, SF_4

55. In which of the following species the interatomic bond angle is 109° 28'? **[2002]**
(a) NH_3, BF_4^- (b) NH_4^+, BF_3
(c) NH_3, BF_4 (d) NH_2^-, BF_3.

56. Hybridisation of the underline atom changes in: **[2002]**

(a) $\underline{Al}H_3$ changes to AlH_4^-

(b) $H_2\underline{O}$ changes to H_3O^+

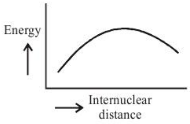
(c) $\underline{N}H_3$ changes to NH_4^+

(d) in all cases

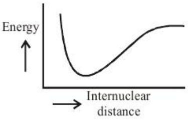
TOPIC 5 Valence Bond and Molecular Orbital Theory

57. The potential energy curve for the H_2 molecule as a function of internuclear distance is : **[Sep. 05, 2020 (I)]**

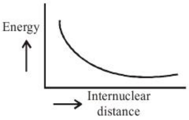
(a)



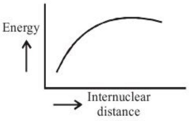
(b)



(c)



(d)



58. The structure of PCl_5 in the solid state is: **[Sep. 05, 2020 (I)]**

(a) tetrahedral $[PCl_4]^+$ and octahedral $[PCl_6]^-$

(b) square planar $[PCl_4]^+$ and octahedral $[PCl_6]^-$

(c) square pyramidal

(d) trigonal bipyramidal

59. Of the species, NO, NO^+, NO^{2+} and NO^-, the one with minimum bond strength is : **[Sep. 03, 2020 (I)]**

(a) NO^+ (b) NO (c) NO^{2+} (d) NO^-

60. If the magnetic moment of a dioxygen species is 1.73 B.M, it may be: **[Jan. 09, 2020 (I)]**

(a) O_2^- or O_2^+ (b) O_2 or O_2^+

(c) O_2 or O_2^- (d) O_2, O_2^- or O_2^+

61. The bond order and the magnetic characteristics of CN^- are: **[Jan. 07, 2020 (II)]**

(a) $2\frac{1}{2}$, diamagnetic (b) 3, diamagnetic

(c) 3, paramagnetic (d) $2\frac{1}{2}$, paramagnetic

62. During the change of O_2 to O_2^-, the incoming electron goes to the orbital : **[April 10, 2019 (I)]**

(a) $\pi 2p_y$ (b) $\sigma^* 2p_z$

(c) $\pi^* 2p_x$ (d) $\pi 2p_x$

63. Among the following, the molecule expected to be stabilised by anion formation is: **[April 9, 2019 (I)]**

C_2, O_2, NO, F_2

(a) C_2 (b) F_2 (c) NO (d) O_2

64. Among the following species, the diamagnetic molecule is: **[April 9, 2019 (II)]**

(a) NO (b) CO (c) B_2 (d) O_2

65. Among the following molecules/ions,

C_2^{2-}, N_2^{2-}, O_2^{2-}, O_2

Which one is diamagnetic and has the shortest bond length? **[April 8, 2019 (II)]**

(a) O_2 (b) N_2^{2-} (c) O_2^{2-} (d) C_2^{2-}

66. Two pi and half sigma bonds are present in: **[Jan. 10, 2019 (I)]**

(a) O_2^+ (b) N_2 (c) O_2 (d) N_2^+

67. According to molecular orbital theory, which of the following is true with respect to Li_2^+ and Li_2^-? **[Jan. 9, 2019 (I)]**

(a) Li_2^+ is unstable and Li_2^- is stable

(b) Li_2^+ is stable and Li_2^- is unstable

(c) Both are stable

(d) Both are unstable

68. In which of the following processes, the bond order has increased and paramagnetic character has changed to diamagnetic? **[Jan. 9, 2019 (II)]**

(a) $NO \rightarrow NO^+$ (b) $N_2 \rightarrow N_2^+$

(c) $O_2 \rightarrow O_2^+$ (d) $O_2 \rightarrow O_2^{2-}$

69. According to molecular orbital theory, which of the following will not be a viable molecule? **[2018]**

(a) He_2^{2+} (b) He_2^+ (c) H_2^- (d) H_2^{2-}

70. $H-N\overset{(I)}{---}N\overset{(II)}{---}N$

In hydrogen azide, the bond orders of bonds (I) and (II) are _________. **[Online April 15, 2018 (I)]**

(a) $I < 2, II > 2$ (b) $I > 2, II > 2$

(c) $I > 2, II < 2$ (d) $I < 2, II < 2$

71. Which of the following best describes the diagram of molecular orbital? **[Online April 15, 2018 (II)]**

(a) A bonding π orbital
(b) A non-bonding orbital
(c) An antibonding σ orbital
(d) An antibonding π orbital

72. In the molecular orbital diagram for the molecular ion, N_2^+, the number of electrons in the σ_{2p} molecular orbital is: **[Online April 15, 2018 (I)]**

(a) 0 (b) 2 (c) 3 (d) 1

73. Which of the following is paramagnetic ? **[Online April 8, 2017]**

(a) NO^+ (b) CO (c) O_2^{2-} (d) B_2

74. Which of the following species is not paramagnetic ? **[2017]**

(a) NO (b) CO (c) O_2 (d) B_2

75. After understanding the assertion and reason, choose the correct option. **[Online April 10, 2015]**

Assertion : In the bonding molecular orbital (MO) of H_2, electron density is increased between the nuclei.

Reason : The bonding MO is $\Psi_A + \Psi_B$, which shows destructive interference of the combining electron waves.

(a) Assertion is incorrect, reason is correct.
(b) Assertion is correct, reason is incorrect.
(c) Assertion and reason are correct and reason is the correct explanation for the assertion.
(d) Assertion and reason are correct, but reason is not the correct explanation for the assertion.

76. Which one of the following properties is **not** shown by NO? **[2014]**

(a) It is diamagnetic in gaseous state
(b) It is neutral oxide
(c) It combines with oxygen to form nitrogen dioxide
(d) Its bond order is 2.5

77. Which one of the following molecules is paramagnetic? **[Online April 19, 2014]**

(a) N_2 (b) NO (c) CO (d) O_3

78. Which of the following has unpaired electron(s)? **[Online April 9, 2014]**

(a) N_2 (b) O_2^- (c) N_2^{2+} (d) O_2^{2-}

79. In which of the following pairs of molecules/ions, both the species are not likely to exist ? **[2013]**

(a) H_2^+, He_2^{2-} (b) H_2^-, He_2^{2-}
(c) H_2^{2+}, He_2 (d) H_2^-, He_2^{2+}

80. Which one of the following molecules is expected to exhibit diamagnetic behaviour ? **[2013]**

(a) C_2 (b) N_2 (c) O_2 (d) S_2

81. Which of the following is the wrong statement **[2013]**

(a) ONCl and ONO^- are not isoelectronic.
(b) O_3 molecule is bent
(c) Ozone is violet-black in solid state
(d) Ozone is diamagnetic gas.

82. Stability of the species Li_2, Li_2^- and Li_2^+ increases in the order of : **[2013]**

(a) $Li_2 < Li_2^+ < Li_2^-$ (b) $Li_2^- < Li_2^+ < Li_2$
(c) $Li_2 < Li_2^- < Li_2^+$ (d) $Li_2^- < Li_2 < Li_2^+$

83. In which of the following ionization processes the bond energy has increased and also the magnetic behaviour has changed from paramagnetic to diamagnetic ? **[Online April 9, 2013]**

(a) $NO \rightarrow NO^+$ (b) $N_2 \rightarrow N_2^+$
(c) $C_2 \rightarrow C_2^+$ (d) $O_2 \rightarrow O_2^+$

84. Bond order normally gives idea of stability of a molecular species. All the molecules viz. H_2, Li_2 and B_2 have the same bond order yet they are not equally stable. Their stability order is **[Online April 22, 2013]**

(a) $H_2 > B_2 > Li_2$ (b) $Li_2 > H_2 > B_2$
(c) $Li_2 > B_2 > H_2$ (d) $B_2 > H_2 > Li_2$

85. The internuclear distances in O – O bonds for O_2^+, O_2, O_2^- and O_2^{2-} respectively are : **[Online April 25, 2013]**

(a) 1.30 Å, 1.49 Å, 1.12 Å, 1.21 Å
(b) 1.49 Å, 1.21 Å, 1.12 Å, 1.30 Å
(c) 1.21 Å, 1.12 Å, 1.49 Å, 1.30 Å
(d) 1.12 Å, 1.21 Å, 1.30 Å, 1.49 Å

86. The number of types of bonds between two carbon atoms in calcium carbide is : **[2011RS]**

(a) One sigma, one pi (b) Two sigma, one pi
(c) Two sigma, two pi (d) One sigma, two pi

87. Using MO theory, predict which of the following species has the shortest bond length? **[2008]**

(a) O_2^+ (b) O_2^- (c) O_2^{2-} (d) O_2^{2+}

88. Which of the following species exhibits the diamagnetic behaviour ? **[2007]**

(a) NO (b) O_2^{2-} (c) O_2^+ (d) O_2

89. In which of the following ionization processes, the bond order has increased and the magnetic behaviour has changed? **[2007]**

(a) $N_2 \rightarrow N_2^+$ (b) $C_2 \rightarrow C_2^+$
(c) $NO \rightarrow NO^+$ (d) $O_2 \rightarrow O_2^+$.

90. Which of the following molecules/ions does not contain unpaired electrons? **[2006]**

(a) N_2^+ (b) O_2 (c) O_2^{2-} (d) B_2

91. Which of the following species is diamagnetic in nature? **[2005]**

(a) H_2^- (b) H_2^+ (c) H_2 (d) He_2^+

92. Which of the following are arranged in an increasing order of their bond strength? **[2002]**

(a) $O_2^- < O_2 < O_2^+ < O_2^{2-}$ (b) $O_2^{2-} < O_2^- < O_2 < O_2^+$
(c) $O_2^- < O_2^{2-} < O_2 < O_2^+$ (d) $O_2^+ < O_2 < O_2^- < O_2^{2-}$

Hints & Solutions

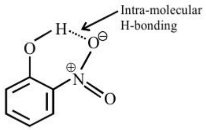
1. **(c)** KCl is an ionic compound while others (PH_3, O_2, B_2H_6, and H_2SO_4) are covalent compounds.

2. **(b)** According to Fajan's rules smaller, highly charged cation has greatest covalent character while large cation with smaller charge has greatest ionic character.

3. **(N)**
   (a) $NO^+ = 7 + 8 - 1 = 14\,e^-$.
   $O_2 = 16\,e^-$
   i.e not isoelectronic.
   (b) Boron forms only covalent compounds. This is due to its extremely high ionisation energy.
   (c) Compounds of Tl^+ are much more stable than those of Tl^{3+}.
   (d) $LiAlH_4$ is a versatile reducing agent in organic synthesis.

4. **(a)** The value of lattice energy depends on the charge present on the two ions and the distance between them.

5. **(b)** Compounds involved in chelation become non-polar. Consequently such compounds are soluble in non-polar solvents like ether, benzene etc. and are only sparingly soluble in water, whereas meta and para isomers are more soluble in water & less soluble in non-polar solvents.



6. **(b)** $NO^-(16)$ – B.O. – 2 $O_2(16)$ – B.O. – 2
   $NO^+(14)$ – B.O. – 3 $NO(15)$ – B.O. – 2.5
   Higher the bond order lower is the bond length. Hence NO^+ will have smallest bond.

7. **(a)** For any species to have same bond order we can expect them to have same number of electrons. Calculating the number of electrons in various species.
   $O_2^-(8+8+1=17)$; $CN^-(6+7+1=14)$
   $NO^+(7+8-1=14)$; $CN^+(6+7-1=12)$
   We find CN^- and NO^+ both have 14 electrons, so they have same bond order.

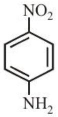
8. **(c)** **Note:** Greater the difference between electronegativity of bonded atoms, stronger will be bond. Since F is most electronegative, hence F – H ...... F is the strongest bond.

9. **(b)** Now since bond order of NO^+ (3) is higher than that of NO (2.5). Thus bond length of NO^+ will be shorter.

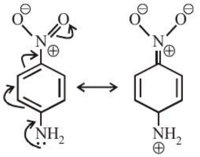
10. **(c)** In ether, there is no H-bonding while alcohols have intermolecular H-bonding.

11. **(d)** $\mu_{CCl_4} = \mu_{CH_4} = 0$ due to symmetrical structure but $\mu_{CHCl_3} \neq 0$. So dipole moment order is :
$$CHCl_3 > CH_4 = CCl_4$$

12. **(c)**



Dipole moment = (Distance between opposite charges) × (charge, q)
$$\mu = q \times d$$
So, greater the distance between the opposite charges higher the dipole. Due to the resonance the greater charge separation occurs between charges due to linearity.



13. **(b)** Dipole moment $(\mu) = q \times d$
$\Rightarrow 1\text{ D} \approx 10^{-18}$ esu cm
0.38×10^{-18} esu cm $= q \times (1.617 \times 10^{-8}\text{cm})$
$q = 2.35 \times 10^{-11}$ esu

So, fractional charge $= \dfrac{\text{Partial charge}}{\text{Total charge}} = \dfrac{q}{Q}$

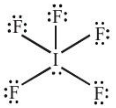
$$= \frac{2.35\times10^{-11}\text{esu}}{4.802\times10^{-10}\text{esu}} = 0.049 \approx 0.05$$

14. **(c)** The bond order of N_2, O_2, and O_2^- are 3, 2 and 1.5 respectively.

Since higher bond order implies higher bond dissociation energy, hence the correct order will be

$$N_2 > O_2 > O_2^-$$

15. **(b)** The geometry of IF_5 is square pyramide with an unsymmetric charge distribution, therefore this molecule is polar.



16. **(d)** Given $e = 1.60 \times 10^{-19}$ C

$d = 9.17 \times 10^{-11}$ m

From $\mu = e \times d$

$\mu = 1.60 \times 10^{-19} \times 9.17 \times 10^{-11}$

$= 14.672 \times 10^{-30}$

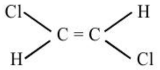
% ionic character

$$= \frac{\text{Observed dipole moment}}{\text{Dipole moment for 100\% ionic bond}}$$

$$= \frac{6.104 \times 10^{-30}}{14.672 \times 10^{-30}} \times 100$$

$= 41.5\%$

17. **(c)**



Dipole moment $(\mu) = 0$

18. **(c)** In nitrogen molecule, both the nitrogen atoms have same electronegativity. So it has zero polarity and hence less tendency to break away and forms ions.

19. **(d)** Smaller the size and higher the charge, more will be the polarising power of the cation. Since the order of the size of cation is $K^+ > Ca^{2+} > Mg^{2+} > Be^{2+}$, so the correct order of polarising power is

$K^+ < Ca^{2+} < Mg^{2+} < Be^{2+}$

20. **(b)** Both NO_2 and O_3 have angular shape and hence will have net dipole moment.

21. **(d)** H_2O - 104.5° (sp^3 with 2 lone pair at O)

NH_3 - 107° (sp^3 with 1 lone pair at N)

CH_4 - 109.5° (sp^3)

H_2S - 92° (sp^3 with 2 lone pair at O)

Lone pair-bond pair repulsion in H_2S will increase because 'S' has lower electronegativity than 'O'. So there will be lesser electron density on 'S' and thus H–S–H bond angle will be smaller than H_2O.

22. **(a)** (a) $[Ni(CN)_4]^{2-} = dsp^2$

(b) $BrF_5 = sp^3d^2$

(c) $XeF_4 = sp^3d^2$

(d) $[CrF_6]^{3-} = d^2sp^2$

23. **(a)** For AB_4 compound possible geometry are

No. of Bond pair	No. of lone pair	Hybridisation
4	0	sp^3
4	1	sp^3d
4	2	sp^3d^2

Structure with sp^3d^2 hybridisation is polar due to lone pair moment while in other possibilities molecules is non-polar. Square pyramidal can be polar due to lone pair moment as the bond pair moments will get cancelled out.

24. **(a)**

(i) XeF_5^- St. No. = Bond pair + Lone Pair

$= (5 + 2) = 7$

So, hybridisation is $= sp^3d^3$

and structure is pentagonal planar.

(ii) XeO_3F_2 St. No. = 5

So, hybridisation is $= sp^3d$

and structure is trigonal bipyramidal.

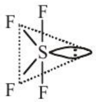
25. **(b)** SF_4

Bond pair = 4

Lone pair = 1

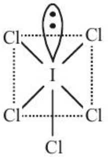
Steric number = 5,

So, hybridisation is sp^3d.



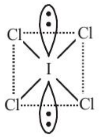
Geometry is trigonal bipyramidal but shape is "See Saw".

26. **(d)** ICl_5 is sp^3d^2 hybridised (5 *bp*, 1 *lp*)



Square pyramidal

ICl_4^- is sp^3d^2 hybridised (4 *bp*, 2 *lp*)

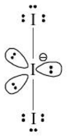


Square planar

27. **(a)**

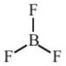
Species	**Hybridisation**
ICl_2^-	sp^3d
ICl_4^-	sp^3d^2
BrF_2^-	sp^3d
IF_6^-	sp^3d^3

28. **(c)**



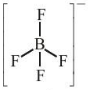
∴ Total number of lone pair of electrons is 9.

29. **(b)** $BF_3 \longrightarrow BF_4^-$



sp^2

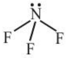
Trigonal planar



sp^3

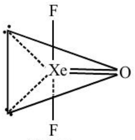
Tetrahedral

30. **(a)**

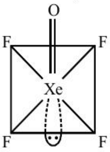


NF_3 has trigonal pyramidal geometry. N atom has one lone pair and three bond pairs of electrons. The electron pair geometry is tetrahedral and molecular geometry is trigonal pyramidal. The bond angles are lower than tetrahedral bond angles due to lone pair - lone pair and lone pair - bond pair repulsions. N atom is sp^3 hybridised.

31. **(d)** $XeOF_2$ $XeOF_4$

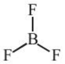


T-shape

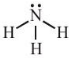


Square pyramidal

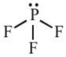
32. **(a)**



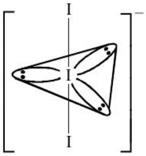
B is sp^2. bond angle = 120°



N is sp^3 with 1 lp, bond angle = 107°



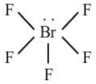
P is sp^3 with 1 lp, when central atom size↑, bond angle↓, $\therefore$ $NH_3 > PF_3$



I is sp^3d (linear), bond angle = 180°

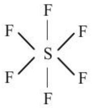
$\therefore$ Dereasing order of bond angle is $I_3^- > BF_3 > NH_3 > PF_3$

33. **(d)** (a) BrF_5



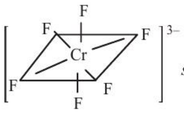
sp^3d^2

(b) SF_6



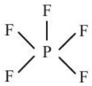
sp^3d^2

(c) $[CrF_6]^{3-}$



sp^3d^2

(d) PF_5



sp^3d

34. **(b)**

	Group	**Hybridisation**	**Shape**	
(a)	BF_3	sp^2	Triangular Planar (T.P.)	
	NF_3	sp^3	Tetrahedral (T)	
	CO_3^{2-}	sp^2	T.P.	
(b)	CO_3^{2-}	sp^2	T.P.	
	NO_3^-	sp^2	T.P.	(All have same hybridisation)
	SO_3	sp^2	T.P.	
(c)	NH_3	sp^3	T	
	SO_3	sp^2	T.P.	
	CO_3^{2-}	sp^2	T.P.	
(d)	NCl_3	sp^3	T	
	BCl_3	sp^2	T.P.	
	SO_3	sp^2	T.P.	

35. **(c)** Hybridisation (H) = [No. of valence electrons of central atom + No. of monovalent atoms attached to it + (–ve charge if any) – (+ve charge if any)]

$NO_2^+ =$ i.e. sp hybridisation

$NO_2^- =$ i.e. sp^2 hybridisation

$NO_3^- =$ i.e. sp^2 hybridisation

The Lewis structure of NO_2 shows a bent molecular geometry with trigonal planar electron pair geometry hence the hybridization will be sp^2.

36. **(d)** $ClF_3 \longrightarrow \text{Hybridisation} = 3 + \frac{1}{2}[7-3] = 5(sp^3d)$

$XeOF_2 \longrightarrow \text{Hybridisation} = 3 + \frac{1}{2}[8-4] = 5(sp^3d)$

$XeF_3^+ \longrightarrow \text{Hybridisation} = 3 + \frac{1}{2}[8-3-1] = 5(sp^3d)$

All molecules have sp^3d hybridisation and 2 lone pairs. Hence all have identical (T-shape).

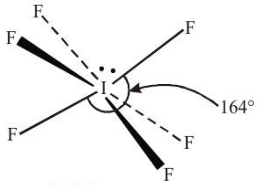
37. **(b)** More the number of lone pairs on central atom, the greater is the contraction caused in the angle between bond pairs. In CH_4 there is no lone pair of electrons, hence bond angle is greatest.

38. **(d)** The structure of CaC_2 is $Ca^{2+}[:C \equiv C:]^{2-}$ i.e, one π and two σ bonds.

39. **(d)** $H \overset{\sigma}{—} C \underset{\pi}{\overset{\pi,\,\sigma}{\equiv}} N$

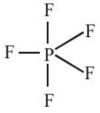
Therefore, HCN has 2 π and 2 σ bonds.

40. **(a)** The structure of IF_6^- is distorted octahedral. This is due to presence of a "weak" lone pair.

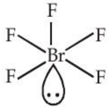


41. **(d)** All have tetrahedral structure.

42. **(c)** PF_5 is trigonal bipyramidal



BrF_5 is square pyramidal (distorted)



43. **(b)** In BF_3, B is sp^2 hybridized with one empty p_z orbital. The empty p_z orbital of BF_3 can be filled by lone pair of molecules such as NH_3. When this occurs a tetrahedral molecule or ion is formed which is sp^3 hybridized.

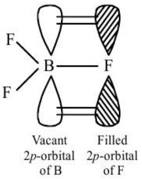
44. **(a)** XeF_4 has square pyramidal structure, while NH_4^+, BF_4^- and CCl_4 have tetrahedral structure.

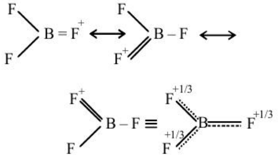
45. **(a)**

Specise	**Hybridisation**	**Shape**
NI_3	sp^3	Trigonal pyramidal
I_3^-	sp^3d	Linear
SO_3^{2-}	sp^3	Trigonal pyramidal
NO_3^-	sp^2	Trigonal planer

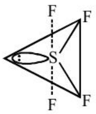
Hence, NI_3 and SO_3^{2-} have same shape.

46. **(b)** **Note:** The delocalised $p\pi - p\pi$ bonding between filled *p*-orbital of F and vacant *p*-orbital of B leads to shortening of B – F bond length which results in higher bond dissociation energy of the B – F bond.





47. **(c)** In SF_4 the hybridisation is sp^3d and the shape of molecule is



It contains two different bonds i.e., axial and equatorial.

48. **(b)** The bond angle decreases on moving down the group due to decrease in bond pair-bond pair repulsion.

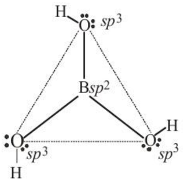
NH_3	PH_3	AsH_3	SbH_3	BiH_3
107°	94°	92°	91°	90°

Note: This can also be explained due to decrease in electronegativity from N to Bi.

49. **(a)** The order of bond angles

$$\underset{120^\circ}{BF_3} > \underset{109^\circ 28'}{SiH_4} > \underset{107^\circ}{NH_3} > \underset{92.5^\circ}{H_2S}$$

50. **(b)**

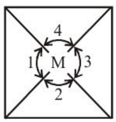


51. **(a)** XeF_4 (sp^3d^2, square planar),

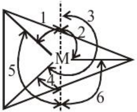
$[Ni(CN)_4]^{2-}$ (dsp^2, square planar),

BF_4^- (sp^3, tetrahedral), SF_4 (sp^3d, see saw shaped)

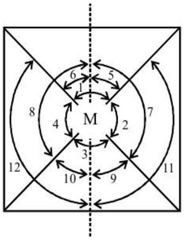
52. **(d)**



dsp^2 hybridisation
Number of 90° angle between bonds = 4



sp^3d or dsp^3 hybridisation
Number of 90° angle between bonds = 6



sp^3d^2 Hybridisation
Number of 90° angle between bonds = 12

53. **(b)** In H_2S, due to low electronegativity of sulphur the *l.p.* - *l.p.* repulsion is more than *b.p.* - *b.p.* repulsion and hence the bond angle is minimum.

	SO_2	H_2O	H_2S	NH_3
Bond angle	119.5°	104.5°	92.5°	106.5°

54. **(a)** Both XeF_2 and CO_2 have a linear structure.
F—Xe—F O=C=O

55. **(a)** In NH_3 and BF_4^-, the hybridisation is sp^3 and the bond angle is almost 109° 28'.

56. **(a)** $\text{Hybridisation} = \frac{1}{2}\left[\begin{pmatrix}\text{No. of electrons}\\ \text{in valence}\\ \text{shell of atom}\end{pmatrix} + \right.$

$$\begin{pmatrix}\text{No.of monovalent}\\ \text{atoms around it}\end{pmatrix} - \begin{pmatrix}\text{Charge on}\\ \text{cation}\end{pmatrix} + \begin{pmatrix}\text{Charge on}\\ \text{anion}\end{pmatrix}$$

(a) For AlH_3,

Hybridisation of Al atom $= \frac{1}{2}[3+3-0+0] = 3 = sp^2$

For AlH_4^-,

Hybridisation of Al atom $= \frac{1}{2}[3+4-0+1] = 4 = sp^3$

(b) For H_2O,
Hybridisation of O atom

$$= \frac{1}{2}[6+2-0+0] = 4 = sp^3$$

For H_3O^+, Hybridisation of O atom

$$= \frac{1}{2}[6+3-1+0] = 4 = sp^3$$

(c) For NH_3,
Hybridisation of N atom

$$= \frac{1}{2}[5+3-0+0] = 4 = sp^3$$

For NH_4^+, Hybridisation of N atom

$$= \frac{1}{2}[5+4-1+0] = 4 = sp^3$$

Thus hybridisation changes only in option (a).

57. **(b)** When two H-atoms come closer then initially due to attraction P.E. is –ve, which decreases more as atoms come closer and after reacting to a minimum value as repulsion starts dominating so, P.E. increases then.

58. **(a)** $2PCl_5\,(s) \longrightarrow \underset{\text{Tetrahedral}}{[PCl_4]^+}\ \underset{\text{Octahedral}}{[PCl_6]^-}$

59. **(d)** Molecular orbital configuration for NO is

$$\sigma 1s^2\, \sigma^* 1s^2\, \sigma 2s^2\, \sigma^* 2s^2\ \pi 2p_x^2\, \pi 2p_y^2\ \sigma 2p_z^2\ \pi^* 2p_z^1$$

Species	Bond order
NO^+	3
NO^{2+}	2.5
NO^-	2
NO	2.5

Bond strength is directly proportional to the bond order, so NO^- has minimum bond strength.

60. **(a)** $\mu = \sqrt{n(n+2)}$ B.M.

$$1.73 = \sqrt{n(n+2)}$$
$$n = 1$$
$$O_2^+ = \sigma 1s^2\, \sigma^* 1s^2\, \sigma 2s^2\, \sigma^* 2s^2\, \sigma 2p_z^{\,2}\, \pi 2p_x^{\,2}$$
$$= \pi 2p_y^{\,2}\, \pi^* 2p_x^{\,1} = \pi^* 2p_y^0$$
$$O_2^- = \sigma 1s^2\, \sigma^* 1s^2\, \sigma 2s^2\, \sigma^* 2s^2\, \sigma 2p_z^{\,2}\, \pi 2p_x^{\,2}$$
$$= \pi 2p_y^{\,2}\, \pi^* 2p_x^{\,2} = \pi^* 2p_y^{\,1}$$

61. **(b)** Total number of electrons in $CN^- = 6 + 7 + 1 = 14$
∴ Molecular orbital distribution

$$\sigma 1s^2\, \sigma^* 1s^2\, \sigma 2s^2\, \sigma^* 2s^2 \begin{bmatrix}\pi 2px^2\\ \pi 2py^2\end{bmatrix} \sigma 2p_z^2$$

$$\therefore \text{Bond order} = \frac{10-4}{2} = 3$$

CN^- is diamagnetic because all electrons are paired.

62. **(c)** Electronic configuration of O_2 is

$$\sigma 1s^2 \sigma^* 1s^2 \sigma 2s^2 \sigma^* 2s^2 \sigma 2p_z^2 \pi 2p_x^2 = \pi 2p_y^2$$
$$\pi^* 2p_x^1 = \pi^* 2p_y^1$$

When an electron is added in O_2 to form O_2^-, the incoming electron goes to $\pi^* 2px$ or $\pi^* 2py$ orbital.

63. **(a)** Configuration of C_2

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

Configuration of C_2^-

$$\sigma 1s^2\, \sigma^* 1s^2\, \sigma 2s^2\, \sigma^* 2s^2\, \pi 2p_x^2 = \pi 2p_y^2\ \sigma 2p_z^1$$

Bond order

$$= \frac{\text{No. of bounding } e^- - \text{No. of antibonding } e^-}{2}$$

C_2 has *s-p* mixing and the HOMO is $\pi 2p_x = \pi 2p_y$ and LUMO is $\sigma 2p_z$. So, the extra electron will occupy bonding molecular orbital and this will lead to increase in bond order. So, C_2^- has more bond order than C_2.

64. **(b)** The molecules with no unpaired electrons are diamagnetic.

Molecule	No. of unpaired electrons
NO	1
CO	Zero
O_2	2
B_2	2

Since CO has no unpaired electron. Hence CO is diamagnetic.

65. **(d)** Bond length $\propto \frac{1}{\text{Bond order}}$

and diamagnetic species has no unpaired electron in their molecular orbitals.

	No. of unpaired electrons	Bond order	Magnetic character
C_2^{2-}	0	3	diamagnetic
N_2^{2-}	2	2	paramagnetic
O_2^{2-}	0	1	diamagnetic
O_2	1	2	paramagnetic

$\therefore$ C_2^{2-} has least bond length and is diamagnetic.

66. **(d)**

$$N_2^+ = 13e^- = \sigma 1s^2 \sigma^* 1s^2 \sigma 2s^2 \sigma^* 2s^2 \pi 2p_x^2 = \pi 2p_y^2 \sigma 2p_z^1$$

$$\text{B.O.} = \frac{\text{Bonding electrons} - \text{Antibonding electrons}}{2}$$

$$\text{B.O.} = \frac{9-4}{2} = 2.5 = 2\pi \text{ bond} + 0.5\,\sigma \text{ bond}$$

67. **(c)** Electronic configuratios of Li_2^+ and Li_2^-:

$Li_2^+ : \sigma 1s^2 \sigma^* 1s^2 \sigma 2s^1$

$Li_2^- : \sigma 1s^2 \sigma^* 1s^2 \sigma 2s^2 \sigma^* 2s^1$

Now,

$$\text{Bond order of } Li_2^+ = \frac{1}{2}(3-2) = \frac{1}{2}$$

$$\text{Bond order of } Li_2^- = \frac{1}{2}(4-3) = \frac{1}{2}$$

Here, both Li_2^+ and Li_2^- have positive bond order, thus both are stable.

68. **(a)** In case of NO (paramagnetic) $\rightarrow$ NO^+ (diamagnetic) the bond order has increased from 2.5 to 3.

For other cases:

N_2 (Diamagnetic) $\rightarrow$ N_2^+ (Paramagnetic)

O_2 (Paramagnetic) $\rightarrow$ O_2^+ (Paramagnetic)

O_2 (Paramagnetic) $\rightarrow$ O_2^{2-} (Diamagnetic)

B.O = 2 B.O = 1

69. **(d)**

Species	No. of e⁻s	Elec. conf.	Bond order
He_2^+	$(4-1=3)$	$\sigma 1s^2 \sigma^* 1s^1$	$\frac{2-1}{2} = 0.5$
H_2^-	$(2+1=3)$	$\sigma 1s^2 \sigma^* 1s^1$	$\frac{2-1}{2} = 0.5$
H_2^{2-}	$(2+2=4)$	$\sigma 1s^2 \sigma^* 1s^2$	$\frac{2-2}{2} = 0$
He_2^{2+}	$(4-2=2)$	$\sigma 1s^2$	$\frac{2-0}{2} = 1$

Molecule having zero bond order will not be a viable molecule.

70. **(a)** As in the resonance structure of hydrogen azide, it can be seen that number of N - N bond for bond (I) ≤ 2.

$$H - \ddot{N} \overset{(I)}{=} \overset{+}{N} \overset{(II)}{=} \underset{\cdot\cdot}{\overset{-}{\ddot{N}}} \longleftrightarrow H - \underset{\cdot\cdot}{\overset{-}{\ddot{N}}} \overset{(I)}{-} \overset{+}{N} \overset{(II)}{\equiv} \ddot{N}$$

Hence for bond (I), bond order will be < 2 whereas for bond (II), number of bond ≥ 2. Thus its bond order will be > 2.

71. **(d)** An antibonding π orbital best describes the given diagram of a molecular orbital. Two orbitals laterally overlap to form π bond. Out of phase combination of these two *p*-orbitals give π^* MO.

72. **(d)** Total electrons in $N_2^+ = (7 \times 2) - 1 = 13$

$$N_2^+ \rightarrow KK\sigma(2s)^2 \sigma^*(2s)^2 \pi(2p_x)^2 = \pi(2p_y)^2 \sigma(2p_z)^1$$

Number of electron in σ_{2p_z} is 1

73. **(d)**

	Total electron
NO^+	14
CO	14
O_2^{2-}	18
B_2	10

$NO^+ \Rightarrow KK \cdot \sigma(2s)^2 \sigma^*(2s)^2 \cdot (\pi 2p_x)^2$

$= (\pi 2p_y)^2 \cdot (\sigma 2p_z)^2$ diamagnetic

$CO \Rightarrow KK \cdot \sigma(2s)^2 \sigma^*(2s)^2 \cdot (\pi 2p_x)^2$

$= (\pi 2p_y)^2 \cdot (\sigma 2p_z)^2$ diamagnetic

$O_2^{2-} \Rightarrow KK \cdot \sigma(2s)^2 \sigma^*(2s)^2 \cdot \sigma(2p_z)^2 (\pi 2p_x)^2$

$= (\pi 2p_y)^2 \cdot \pi^*(2p_x)^2 = \pi^*(2p_y)^2$

diamagnetic

$B_2 \Rightarrow KK \cdot \sigma(2s)^2 \sigma^*(2s)^2 \cdot \pi(2p_x)^1 = \pi(2p_y)^1$

paramagnetic

74. **(b)**

(a) NO $\rightarrow$ One unpaired electron is present in π^* molecular orbit, hence paramagnetic.

(b) CO (14) $\rightarrow$ $KK\sigma 2s^2 \pi 2p_x^2 = \pi 2p_y^2 \sigma 2p_z^2 \sigma^* 2s^2$

No unpaired electron, hence diamagnetic.

(c) $O_2(16) \rightarrow$

$KK\sigma 2s^2 \sigma^* 2s^2 \sigma 2p_z^2 \pi 2p_x^2 = \pi 2p_y^2 \pi^* 2p_x^1 = \pi^* 2p_y^1$

Two unpaired electrons, hence paramagnetic.

(d) $B_2(10) \rightarrow KK\,\sigma 2s^2 \sigma^* 2s^2 \pi 2p_x^1 = \pi 2p_y^1$

B_2 contains two unpaired electrons, hence paramagnetic.

75. **(b)** Assertion is correct but reason is incorrect. Bonding MO shows constructive interference of the combining electron waves.

76. **(a)** Nitric oxide is paramagnetic in the gaseous state because of the presence of one unpaired electron in its outermost shell.

The electronic configuration of NO is

$\sigma KK\sigma 2s^2\, \sigma^* 2s^2 \sigma 2p_z^2\, \pi 2p_x^2 = \pi 2p_y^2 \pi^* 2p_x^1 = \pi^* 2p_y^0$

77. **(b)** The molecular orbital configuration of the molecules given is

Total no. of electrons in NO = 7(N) + 8(O) = 15

Hence E.C. of NO = $KK\sigma(2s)^2 \sigma^*(2s)^2 \sigma 2p_z{}^2$

$\pi(2p_x)^2 \pi(2p_y)^2 \pi^*(2p_x)^1$

Due to presence of one unpaired electron NO is paramagnetic. Except NO all are diamagnetic due to absence of unpaired electrons.

78. **(b)** $O_2^-(17) = KK(\sigma 2s)^2 (\sigma^* 2s^2)(\sigma 2p_z)^2$

$(\pi 2p_x)^2 = (\pi 2p_y)^2 (\pi^* 2p_x)^2 = (\pi^* 2p_y)^1$

One unpaired electron - paramagnetic.

79. **(c)** $H_2^{2+} = \sigma 1s^0 \sigma^* 1s^0$

Bond order for $H_2^{2+} = \frac{1}{2}(0-0) = 0$

$He_2 = \sigma 1s^2 \sigma^* 1s^2$

Bond order for $He_2 = \frac{1}{2}(2-2) = 0$

So both H_2^{2+} and He_2 do not exist.

80. **(a, b)** The molecular orbital structures of C_2 and N_2 are

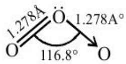
$N_2 = KK\,\sigma 2s^2\, \sigma^* 2s^2 \pi 2p_x^2 = \pi 2p_y^2\, \sigma 2p_z^2$

$C_2 = KK\,\sigma 2s^2\, \sigma^* 2s^2 \pi 2py_x^2 = \pi 2p_y^2$

Both N_2 and C_2 have paired electrons, hence they are diamagnetic.

81. **(N)** All options are correct,

(a) $\left.\begin{array}{l} ONCl = 8+7+17 = 32e^- \\ ONO^- = 8+7+8+1 = 24e^- \end{array}\right\}$ not isoelectronic

(b) 

The central atom is sp^2 hybridised with one lone pair.

(c) It is a pale blue gas. At – 249.7°, it forms violet black crystals.

(d) It is diamagnetic in nature due to absence of unpaired electrons.

82. **(b)** $Li_2 = \sigma 1s^2\, \sigma^* 1s^2\, \sigma 2s^2$

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

$Li_2^+ = \sigma 1s^2\, \sigma^* 1s^2\, \sigma 2s^1$

B.O. $= \frac{1}{2}(3-2) = 0.5$

$Li_2^- = \sigma 1s^2\, \sigma^* 1s^2 \sigma 2s^2 \sigma^* 2s^1$

B.O. $= \frac{1}{2}(4-3) = 0.5$

The bond order of Li_2^+ and Li_2^- is same but Li_2^+ is more stable than Li_2^- because Li_2^+ is smaller in size and has 2 electrons in antibonding orbitals whereas Li_2^- has 3 electrons in antibonding orbitals. Hence Li_2^+ is more stable than Li_2^-.

83. **(a)** For NO

Total no. of electrons = 15

B.O = 2.5

Mag. behaviour = paramagnetic

For NO^+

Total no. of electrons = 14

B.O = 3

Mag. behaviour = diamagnetic

84. **(N)** None of the given option is correct.

The molecular orbital configuration of the given molecules is

$H_2 = \sigma 1s^2\, \sigma 1s^0$ (no anti-bonding electron)

$Li_2 = \sigma 1s^2\, \sigma^* 1s^2\, \sigma 2s^2$(two anti-bonding electrons)

$B_2 = \sigma 1s^2\, \sigma^* 1s^2\, \sigma 2s^2\, \sigma^* 2s^2 \left\{\pi 2p_y^1 = \pi 2p_z^1\right\}$

(4 anti-bonding electrons)

Though the bond order of all the species are same (B.O = 1) but stability is different. This is due to difference in the presence of no. of anti-bonding electron.

Higher the no. of anti-bonding electron lower is the stability hence the correct order is $H_2 > Li_2 > B_2$

85. **(d)** The bond length follows the order

$$O_2^+ < O_2 < O_2^- < O_2^{2-}$$

According to this the possible values are
1.12Å, 1.21Å, 1.30Å, 1.49Å

86. **(d)** Calcium carbide exists as Ca^{2+} and C_2^{2-}. According to the molecular orbital model, C_2^{2-} should have following molecular orbital configuration :

$KK\ \sigma 2s^2\ \sigma^* 2s^2\ \pi 2p_x^2 = \pi 2p_y^2\ \sigma 2p_z^2$

Thus M.O. configuration suggests that it contains one σ & two π bonds.

87. **(d)** Bond order

$$= \frac{\text{No. of bonding electrons} - \text{No. of antibonding electrons}}{2}$$

Bond order in $O_2^+ = \frac{10-5}{2} = 2.5$

Bond order in $O_2^- = \frac{10-7}{2} = 1.5$

Bond order in $O_2^{2-} = \frac{10-8}{2} = 1$

Bond order in $O_2^{2+} = \frac{10-4}{2} = 3$

Since, bond order $\propto \frac{1}{\text{Bond length}}$

$\therefore$ Bond length is shortest in O_2^{2+}.

88. **(b)** Diamagnetic species have no unpaired electrons whereas paramagnetic species has one or more unpaired electrons.
For electronic configuration of O_2^+, O_2 and O_2^{2-}, consult Q. 2. O_2 and O_2^+ have 2 and 1 unpaired electron respectively, while O_2^{2-} has no unpaired electron

$NO \rightarrow KK\sigma 2s^2 \sigma^* 2s^2 \sigma 2p_z^2\ \pi 2p_x^2 = \pi 2p_y^2$

$\pi^* 2p_x^1 = \pi^* 2p_y^0$

Thus no has one unpaired electron

89. **(c)** (a) N_2 : bond order 3, diamagnetic
N_2^+ : bond order 2.5, paramagnetic
(b) C_2 : bond order 2, diamagnetic
C_2^+ : bond order 1.5, paramagnetic
(c) NO : bond order 2.5, paramagnetic
NO^+ : bond order 3, diamagnetic
(d) O_2 : bond order 2, paramagnetic
O_2^+ : bond order 2.5, paramagnetic

90. **(c)** The distribution of electrons in MOs is as follows :

N_2^+(electrons 13) $\Rightarrow KK\sigma 2s^2 \sigma^* 2s^2 \sigma 2p_z^2 \pi 2p_x^2 = \pi 2p_y^1$

$\Rightarrow KK\ \sigma 2s^2\ \sigma^* 2s^2\ \sigma 2p_x{}^2 \Rightarrow O_2$ (electron 16)
$\pi 2p_x^2 = \pi 2p_y{}^2\ \pi^* 2p_x^1 = \pi^* 2p_y^1$

$\Rightarrow KK\ \sigma 2s^2\ \sigma^* 2s^2\ \sigma 2p_x{}^2 \Rightarrow O_2^{2-}$ (electron 18)
$\pi 2p_x^2 = \pi 2p_y^2\ \pi^* 2p_x^2 = \pi^* 2p_y{}^2$

B_2 (electrons 10) $\Rightarrow KK\ \sigma 2s^2\ \sigma^* 2s^2\ \sigma 2p_x{}^2$
$KK\ \sigma 2s^2\ \sigma^* 2s^2\ \pi 2p_x^1 = \pi 2p_y^1$

Only O_2^{2-} does not contain any unpaired electron.

91. **(c)** A diamagnetic substance contains no unpaired electron. H_2 is diamagnetic as it contains all paired electrons

$H_2 = \sigma 1s^2$, $H_2^+ = \sigma 1s^1$, $H_2^- = \sigma 1s^2 \sigma 1s$
(diamagnetic) (paramagnetic) (paramagnetic)

$He_2^+ = \sigma 1s^2 \sigma^* 1s$
(paramagnetic)

92. **(b)** $O_2{}^+(15)$

$= KK\ \sigma 2s^2\ \sigma^* 2s^2\ \sigma 2p_z{}^2\ \pi 2p_x^2 = \pi 2p_y^2\ \pi^* 2p_x^1 = \pi 2p_y^0$

Bond order $= \frac{1}{2}(8-3) = \frac{5}{2} = 2.5$

$O_2(16) = KK\ \sigma 2s^2\ \sigma^* 2s^2\ \sigma 2p_z^2\ \pi 2p_x{}^2 = \pi 2p_y^2\ \pi^* 2p_x{}^1 = \pi^* 2p_y{}^1$

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

$O_2{}^-(17) = KK\ \sigma 2s^2\ \sigma^* 2s^2\ \sigma 2p_z{}^2\ \pi 2p_x{}^2 = \pi 2p_y{}^2\ \pi^* 2p_x{}^2 = \pi^* 2p_y{}^1$

Bond order $= \frac{1}{2}(8-5) = 1.5$

$O_2{}^{2-}(18) = KK\ \sigma 2s^2\ \sigma^* 2s^2\ \sigma 2p_z{}^2\ \pi 2p_x{}^2 = \pi 2p_y{}^2\ \pi^* 2p_x{}^2 = \pi^* 2p_y{}^2$

Bond order $= \frac{1}{2}(8-6) = 1$

Note: As we know that as the bond order decreases, stability also decreases and hence the bond strength also decreases. Therefore the correct order of their increasing bond strength is

$$O_2^{2-} < O_2^- < O_2 < O_2^+$$