Exercise-1

Marked questions are recommended for Revision.

PART - I : SUBJECTIVE QUESTIONS

Section (A) : MOT

A-1. Find out the bond order of :
(a) H_2 (b) H_2^+ (c) He_2 (d) Li_2 (e) Be_2 (f) B_2

A-2. Identify the molecules or atoms or ions from the following molecular orbital energy level formulations. The species should be selected from (B_2, C_2, O_2^{2+}, O_2, F_2, N_2)

(a) KK $\sigma(2s)^2\ \sigma^*(2s)^2\pi(2p_x)^1\ \pi(2p_y)^1$

(b) KK $\sigma(2s)^2\ \sigma^*(2s)^2\pi(2p_x)^2\ \pi(2p_y)^2$

(c) KK $\sigma(2s)^2\ \sigma^*(2s)^2\ \sigma(2p_z)^2\pi(2p_x)^2\ \pi(2p_y)^2$

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

(e) KK $\sigma(2s)^2\ \sigma^*(2s)^2\sigma(2p_z)^2\pi(2p_x)^2\ \pi(2p_y)^2\pi^*(2p_x)^2\pi^*(2p_y)^2$

(f) KK $\sigma(2s)^2\ \sigma^*(2s)^2\pi(2p_y)^2\pi(2p_x)^2\sigma(2p_z)^2$

A-3. What is the bond order of underlined species in <u>NO</u> [BF_4]?

Section (B) : Applilcation of MOT

B-1. How would you explain that B_2 molecule is not diamagnetic?

B-2. Explain why NO^+ is more stable towards dissociation into its atoms than NO ?

B-3. Which of the following are gerade molecular orbitals?
(i) σ^*2s (ii) $\sigma2p_z$ (iii) $\pi2p_y$ (iv) π^*2p_x

B-4. Arrange following compounds in the order of increasing order of O–O bond length.
(i) O_2 (ii) $O_2[BF_4]$ (iii) KO_2

Section (C) : Metallic bonding

C-1. Zinc has lowest melting point in 3d-series elements. Why ?

C-2. Among Be and Li, which should have higher melting point and why ?

PART - II : ONLY ONE OPTION CORRECT TYPE

Section (A) : MOT

A-1. During the formation of a molecular orbital from atomic orbitals of the same atom, probability of electron density is :
(A) none zero in the nodal plane (B) maximum in the nodal plane
(C) zero in the nodal plane (D) zero on the surface of the lobe

A-2. If Z-axis is the molecular axis, then π-molecular orbitals are formed by the overlap of
(A) $s + p_z$ (B) $p_x + p_y$ (C) $p_z + p_z$ (D) $p_x + p_x$

A-3. Bond order is a concept in the molecular orbital theory. It depends on the number of electrons in the bonding and antibonding orbitals. Which of the following statements is true about it ? The bond order
(A) Can have a negative quantity
(B) Has always an integral value
(C) Can assume any positive or integral or fractional value including zero
(D) Is a non zero quantity

A-4. Which of the following pairs have identical values of bond order ?
(A) N_2^+ and O_2^+ (B) F_2 and Ne_2 (C) O_2 and B_2 (D) C_2 and N_2

A-5. Which of the following molecules/ions exhibit sp mixing?
(A) B_2 (B) C_2^{2-} (C) O_2^+ (D) Both (A) and (B)

A-6. The common features of the species N_2^{2-} , O_2 and NO^- are :
(A) bond order three and isoelectronic. (B) bond order two and isoelectronic.
(C) bond order three but not isoelectronic. (D) bond order two but not isoelectronic.

A-7. Which of the following molecular orbitals has two nodal planes.
(A) $\sigma 2s$ (B) $\pi 2p_y$ (C) $\pi^* 2p_y$ (D) $\sigma^* 2p_x$

Section (B) : Applilcation of MOT

B-1. Among the following species, which has the minimum bond length ?
(A) B_2 (B) C_2 (C) F_2 (D) O_2^-

B-2. Which of the following species is paramagnetic ?
(A) NO^- (B) O_2^{2-} (C) CN^- (D) CO

B-3. The following molecules / species have been arranged in the order of their increasing bond orders, Identify the correct order.
(I) O_2 (II) O_2^- (III) O_2^{2-} (IV) O_2^+
(A) I I I < I I < I < IV (B) IV < I I I < I I < I (C) I I I < I I < IV < I (D) I I < I I I < I < IV

B-4. Which one is paramagnetic from the following
(A) O_2^- (B) NO (C) Both (A) and (B) (D) CN^-

B-5. Which of the following orders is correct in respect of bond dissociation energy ?
(A) $N_2^+ > N_2^-$ (B) $O_2^+ > O_3$ (C) $NO^+ > NO$ (D) All of these

B-6. S_1 : The HOMO in F_2^- is $\pi^* 2p_x = \pi^* 2p_y$ molecular orbitals.
S_2 : Bond order of O_2^- is more then O_2^+.
S_3 : NO^+ is more stable than N_2^+.
S_4 : C_2 is more stable than C_2^+.
State, in order, whether S_1, S_2, S_3, S_4 are true or false
(A) FFFT (B) FTTT (C) FTFT (D) FFTT

Section (C) : Metallic bonding

C-1. Iron is harder than sodium because :
(A) iron atoms are smaller. (B) iron atoms are more closely packed.
(C) metallic bonds are stronger in sodium. (D) metallic bonds are stronger in iron.

C-2. The enhanced force of cohesion in metals is due to :
(A) The covalent linkages between atoms
(B) The electrovalent linkages between atoms
(C) The lack of exchange of valency electrons
(D) The delocalization of valence electron between metallic kernels.

C-3. In the following metals which one has lowest probable interatomic forces
(A) Copper (B) Silver (C) Zinc (D) Mercury

PART - III : MATCH THE COLUMN

1. Match the following :

	Column – I		**Column – II**
(A)	O_2 and NO^-	(p)	Same magnetic property and bond order as that in N_2^+
(B)	O_2^+ and NO	(q)	Same bond order but not same magnetic property as that in O_2
(C)	CO and CN^-	(r)	Same magnetic property and bond order as that N_2^{2-}
(D)	C_2 and CN^+	(s)	Same magnetic property and bond order as that in NO^+

Exercise-2

Marked questions are recommended for Revision.

PART - I : ONLY ONE OPTION CORRECT TYPE

1. Number of antibonding electrons in N_2 is :
(A) 4 (B) 10 (C) 12 (D) 14

2. Following is the molecular orbital configuration of a diatomic molecule

$$\sigma 1s^2\ \sigma^* 1s^2\ \sigma 2s^2\ \sigma^* 2s^2\ \sigma 2p_x^2 \begin{cases} \pi 2p_y^2 \\ \pi 2p_z^2 \end{cases}$$

Its bond order is :
(A) 3 (B) 2.5 (C) 2 (D) 1

3. The bond order of He_2^+ molecule ion is :
(A) 1 (B) 2 (C) 1/2 (D) 1/4

4. Which species can exist among the following :
(A) B_2 (B) Be_2 (C) Ne_2 (D) He_2

5. Among the following which one will have the largest O – O bond length ?
(A) KO_2 (B) O_2 (C) $O_2^+[AsF_6]^-$ (D) K_2O_2

6. The correct order in which the O–O bond length increases in the following is :
(A) $H_2O_2 < O_2 < O_3$ (B) $O_2 < H_2O_2 < O_3$ (C) $O_2 < O_3 < H_2O_2$ (D) $O_3 < H_2O_2 < O_2$

7. Which of the following is a **<u>wrong</u>** order with respect to the property mentioned against each ?
(A) $O_2^{2-} > O_2 > O_2^+$ [Paramagnetic moment] (B) $(NO)^- > (NO) > (NO)^+$ [bond length]
(C) $H_2 > H_2^+ > He_2^+$ [bond energy] (D) $NO_2^+ > NO_2 > NO_2^-$ [bond angle]

8. Which of the following option with respect to increasing bond dissociation energies is correct ?
(A) $NO < C_2 < O_2^- < He_2^+$ (B) $C_2 < NO < He_2^+ < O_2^-$
(C) $He_2^+ < O_2^- < NO < C_2$ (D) $He_2^+ < O_2^- < C_2 < NO$

9. Pick out the incorrect statement.
(A) N_2 has greater dissociation energy than N_2^+ (B) O_2 has lower dissociation energy than O_2^+
(C) Bond length in N_2^+ is less than N_2 (D) Bond length in NO^+ is less than in NO.

10. The species which are diamagnetic :
(A) O_2^- (B) NO_2 (C) ClO_2 (D) N_2O_4

11. Which of the following is observed in metallic bonds ?
(A) Mobile valence electrons (B) Localised electrons
(C) Highly directed bond (D) None of these

PART - II : SINGLE OR DOUBLE INTEGER TYPE

1. Find the no. of species having fractional bond order ?
(a) N_2^+ (b) N_2^- (c) O_2 (d) O_2^+
(e) F_2 (f) B_2 (g) C_2^+ (h) CN^- (i) NO^+

2. Find out the no. of correct statements :
(a) Bond length N_2^+ > Bond length N_2 (b) Bond length NO^+ < Bond length of NO
(c) Bond length CN^- < Bond length of CN (d) Bond length O_2^- < Bond length of O_2^{-2}
(e) Bond length O_2 > Bond length of O_2^+ (f) Bond length B_2 > Bond length of B_2^-

3. In how many conversions, the bond length increases ?
(i) $NO \longrightarrow NO^+$ (ii) N_2^+ N_2^- (iii) $O_2 \longrightarrow O_2^+$ (iv) $H_2 \longrightarrow H_2+$
(v) $NH_3 \longrightarrow NH_4^+$ (vi) $NH_3 \longrightarrow NH_2^-$ (vii) $BF_3 \longrightarrow BF_4^-$

4. Which of the following have bond order less than two ?
(a) NO_3^- (b) CO_3^{2-} (c) F_2 (d) Cl_2
(e) Br_2 (f) O_2^{2-} (g) O_2^- (h) N_2^-
(i) O_2^{2+} (j) Li_2^+ (k) He_2^+

PART - III : ONE OR MORE THAN ONE OPTIONS CORRECT TYPE

1. Which of the following have bond order three ?
(A) O_2^{2+} (B) NO^+ (C) CN^- (D) CN^+

2. The species which are paramagnetic is/are :
(A) NO (B) NO_2 (C) ClO_2 (D) N_2O_4

3. Which of the statement(s) are correct ?
(A) There is a single bond in FO^+
(B) The F and O are further apart in FO^- than in FO^+.
(C) There is a double bond in FO^-.
(D) It would take more energy to break F–O bond in FO^+ than in FO^-.

4. Among the following, the species with one unpaired electron are :
(A) O_2^+ (B) NO (C) O_2^- (D) B_2

5. Identify correct statements
(A) Down the group strength of metallic bond increases nearly all in transition elements.
(B) Down the group strength of metallic bond increases in alkali metals.
(C) Down the group strength of metallic bond decreases in alkali metals.
(D) Down the group strength of metallic bond decreases in transition metals.

6. Which of the following statements are correct for band theory of metallic bond.
(A) Valence band is empty or half filled in metal.
(B) Conduction band is empty in metal
(C) Energy gap between conduction and valence band is very large in non-conductors.
(D) Overlapping of conduction & valence band occurs in semi-conductors

7. The force that binds a metal atom to a number of electrons with in its sphere of influence is known as a metallic bond. Now, which of these is /are true for this found.
(A) Metallic bond is non-directional in nature.
(B) Metallic bonds are weaker than covalent bond.
(C) Energy required to vapourise a mole of metal (say, copper) to the vapour state is larger than the energy required to vapourise a mole of a covalent substance (say, graphite)
(D) The valency electrons in a metallic bond are mobile.

PART - IV : COMPREHENSION

Read the following passage carefully and answer the questions.
Comprehension # 1

The distribution of electrons among various molecular orbitals is called the electronic configuration of the molecule which provides us the following very important informations about the molecule .
(A) Stability of molecule : The molecule is stable if number of bonding molecular orbital electrons (N_b) is greater than the number of antibonding molecular orbital electrons (N_a) and vice- versa.

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

A positive bond order means a stable molecule while a negative or zero bond order means an unstable molecule.
(C) Nature of the bond : Bond order 1, 2,or 3 corresponds to single, double or triple bonds respectively.
(D) Bond length : Bond length decreases as bond order increases.
(E) Magnetic nature : Molecular orbitals in a molecule are doubly occupied, the substance is diamagnetic and if one or more molecular orbitals are singly occupied, it is paramagnetic.

1. Which of the following statements is incorrect ?
(A) Among O_2^+, O_2 and O_2^- the stability decreases as $O_2^+ > O_2 > O_2^-$
(B) He_2 molecule does not exit as the effect of bonding and anti-bonding molecular orbitals cancel each other
(C) C_2, O_2^{2-} and Li_2 are diamagnetic
(D) In F_2 molecule, the energy of $\sigma 2P_z$ is more than π_{2px} and π_{2Py}

2. The bromine (Br_2) is coloured because:
(A) the difference in energy (ΔE) between HOMO and LUMO is large and the electronic excitation take place by absorption of light which falls in ultra violet region.
(B) the difference in energy (ΔE) between HOMO and LUMO is small and the electronic excitation take place by absorption of light which falls in infrared region.
(C) the bromine molecule is paramagnetic and the difference in energy (ΔE) is such that the electronic excitation take place in visible light.
(D) the difference in energy (ΔE) between HOMO and LUMO is such that the electronic excitation take place by absorption of light which falls in visible region and bromine molecule is diamagnetic.

3. N_2 has greater bond dissociation energy than N_2^+ , where as O_2 has a lower bond dissociation energy than O_2^+ because:
(A) Bond order is reduced when O_2 is ionized to O_2^+ and bond order is increased when N_2 is ionized to N_2^+
(B) Bond order is increased when O_2 is ionized to O_2^+ and bond order is decreased when N_2 is ionized to N_2^+
(C) Bond order is deceased when O_2 is ionized to O_2^+ and bond order is decreased when N_2^- is ionized to N_2^+
(D) None of these.

Comprehension # 2

In a molten metal, the metallic bond is still present, although the order structure has been broken down. The metallic bond isn't fully broken until the metal boils. That means boiling point is actually a better guide to the strength of the metallic bond then melting point is. On melting the bond is loosened, not broken.

4. Order of boiling point of K, Ca, Sc is
(A) K > Ca > Sc (B) Ca > K > Sc (C) Sc > Ca > K (D) K > Sc > Ca

5. Order of boiling point & melting point of Zn, Cd, Hg, respectively is :
(A) Zn > Cd > Hg & Zn > Cd > Hg (B) Hg > Cd > Zn & Zn > Cd > Hg
(C) Hg > Cd > Zn & Hg > Cd > Zn (D) Zn > Cd > Hg & Hg > Cd > Zn

Comprehension # 3

Two models are considered to explain metallic bonding :
(A) Band model (B) Electron-sea model

(A) Band Model :

The interaction of two atomic orbitals, say the 3s-orbitals of two sodium atoms, produces two molecular orbitals, one bonding orbital and one antibonding orbital. If N atomic orbitals interact, N molecular orbitals are formed. Atoms interact more strongly with nearby atoms than with those farther away. The energy that separates bonding and antibonding molecular orbitals decreases as the interaction (overlap) between the atomic orbitals decreases. When we consider all the possible interactions among one mole of Na atoms, there is formation of series of very closely spaced molecular orbitals ($3\sigma s$ and $3\sigma^* s$). This consists of a nearly continuous band of orbitals belonging to the crystal as a whole. One mole of Na atoms contributes one mole (6.02×10^{23}) of valence electrons thus, 6.02×10^{23} orbitals in the band are half-filled.

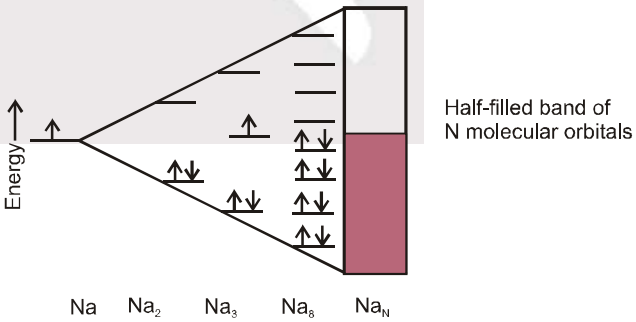


Figure-1. The band of orbitals resulting from interaction of the 3s-orbitals in a crystal of sodium

The empty 3 p atomic orbitals of Na atoms also interact to form a wide band of $3 \times 6.07 \times 10^{23}$ orbitals.

The 3s and 3p atomic orbitals are quite close in energy, so that these bands of molecular orbitals overlap. The two overlapping bands contain $4 \times 6.02 \times 10^{23}$ orbitals. Because each orbital can hold two electrons, the resulting combination of bands is only one-eighth full.

According to band theory, the highest-energy electrons of metallic crystals occupy either a partially filled band or a filled band that overlaps an empty band. A band within which (or into which) electrons must move to allow electrical conduction is called a conduction band. The electrical conductivity of a metal decreases as temperature increases. The increase in temperature causes thermal agitation of the metal ions. This impedes the flow of electrons when an electric field is applied.

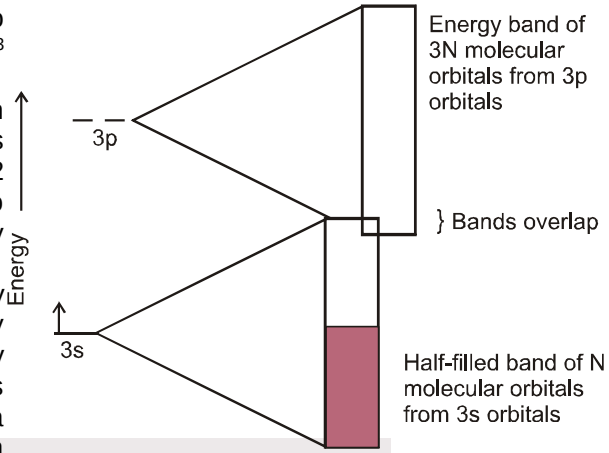


Figure-2. Overlapping of a half–filled "3s" band with an empty "3p" band of Na_N crystal

Crystalline non-metals, such as diamond and phosphorus, are insulators, they do not conduct electricity. It is due to the fact that their highest-energy electrons occupy filled bands of molecular orbitals that are separated from the lowest empty bond (conduction band) by an energy difference called the band gap. In an insulator, this band gap is an energy difference that is too large for electrons to jump to get to the conduction band.

Elements that are semiconductors have filled bands that are only slightly below, but do not overlap with empty bands. They do not conduct electricity at low temperatures, but a small increase in temperature is sufficient to excite some of the highest-energy electrons into the empty conduction band.

(B) Electron-Sea Model :

Metals have ability to conduct electricity, ability to conduct heat, ease of deformation [that is, the ability to be flattened into sheets (malleability) and to be drawn into wires (ductility)] and lustrous appearance.

One over simplified model that can account for some of these properties is the electron-sea model. The metal is pictured as a network of positive ions immersed in a "sea of electrons". In lithium the ions would be Li^+ and one electron per atom would be contributed to the sea. These free electrons account for the characteristic metallic properties. If the ends of a bar of metal are connected to a source of electric current, electrons from the external source enter the bar at one end. Free electrons pass through the metal and leave the other end at the same rate.

In thermal conductivity no electrons leave or enter the metal but those in the region being heated gain kinetic energy and transfer this to other electrons.

According to the electron-sea model, the case of deformation of metals can be thought of in this way : If one layer of metal ions is forced across another, perhaps by hammering, the internal structure remains unchanged as the sea of electrons rapidly adjusts to the new situation.

6. Considering band model, select the incorrect statement :
(A) Li metal should have partilly filled valence band and empty conduction band.
(B) Mg metal should have fully filled valence band and overlapping conduction band.
(C) Electrical conductivity of a metal decreases as temperature increases.
(D) The energy spread of each atomic energy level of an element behaving like a semiconductor is infinitisimally small.

7. All metal written below have usually low melting points except :
(A) Caesium (B) Gallium (C) Gold (D) Mercury

8. Which of the following physical properties can be explained by electron sea model :
(A) Electrical conduction (B) Thermal conduction
(C) Malleability (D) All of these

Comprehension # 4

Answer Q.9, Q.10 and Q.11 by appropriately matching the information given in the three columns of the following table.

Observe the three columns in which column-1 represents molecule, column-2 represents bond orders while column-3 represents molecule properties. Properties of molecule explained by molecular orbital theory. Like megnatic nature, orbital mixing etc.

Column 1	Column 2	Column 3
(I) B_2	(i) Bond Order = 2	(P) Diamagnetic in Nature
(II) O_2^+	(ii) Bond Order = 2.5	(Q) SP Mixing Occure
(III) F_2	(iii) Bond Order = 1	(R) Paramagnetic in Nature
(IV) C_2	(iv) Bond Order = 3	(S) Highest Occupied Molecular orbital (HOMO) is Bonding Molecular orbital (BMO)

9. Which is incorrect combination?
(A) (I) (iii) (Q) (B) (II) (ii) (P) (C) (III) (iii) (P) (D) (IV) (i) (P)

10. Which is correct combination for Diamagnetic species ?
(A) (III) (i) (P) (B) (IV) (ii) (R) (C) (IV) (i) (S) (D) (III) (iii) (Q)

11. Which is correct combination?
(A) (III) (ii) (S) (B) (III) (iii) (Q) (C) (II) (ii) (P) (D) (I) (iii) (R)

Exercise-3

*** Marked Questions may have more than one correct option.**

PART - I : JEE (ADVANCED) / IIT-JEE PROBLEMS (PREVIOUS YEARS)

1. Write the Molecular orbital electron distribution of O_2. Specify its bond order and magnetic property. **[JEE–2000(M), 3/135]**

2. Which of the following molecular species has unpaired electron(s) ? **[JEE–2002(S), 3/150]**
(A) N_2 (B) F_2 (C) O_2^- (D) O_2^{2-}

3. According to molecular orbital theory, which one of the following statements about the molecular species O_2^+ is correct ? **[JEE–2004(S), 3/144]**
(A) It is paramagnetic and has less bond order than O_2
(B) It is paramagnetic and more bond order than O_2
(C) It is diamagnetic and has less bond order than O_2
(D) It is diamagnetic and has more bond order than O_2

4. Arrange the following three compounds in terms of increasing O—O bond length :
O_2, O_2 $[AsF_6]$, K $[O_2]$
Justify your answer based on the ground state electronic configuration of the dioxygen species in these three compounds. **[JEE–2004(M), 2/144]**

5. The species having bond order different from that in CO is : **[JEE–2007, 3/162]**
(A) NO^- (B) NO^+ (C) CN^- (D) N_2

6. Among the following, the paramagnetic compound is : **[JEE–2007, 3/162]**
(A) Na_2O_2 (B) O_3 (C) N_2O (D) KO_2

7. **Statement-1 :** Band gap in germanium is small, **because**
Statement-2 : The energy spread of each germanium atomic energy level is infinitesimally small. **[JEE–2007, 3/162]**
(A) Statement-1 is true, statement-2 is true; statement-2 is a correct explanation for statement-1.
(B) Statement-1 is true, statement-2 is true; statement-2 is NOT a correct explanation for statement-1.
(C) Statement-1 is true, statement-2 is false.
(D) Statement-1 is false, statement-2 is true.

8. **Statement-1 :** Boron always forms covalent bond, **because**
Statement-2 : The small size of B^{3+} favours formation of covalent bond. **[JEE–2007, 3/162]**
(A) Statement-1 is True, Statement-2 is True; Statement-2 is a correct explanation for Statement-1.
(B) Statement-1 is True, Statement-2 is True; Statement-2 is NOT a correct explanation for Statement-1.
(C) Statement-1 is True, Statement-2 is False.
(D) Statement-1 is False, Statement-2 is True.

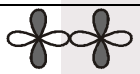
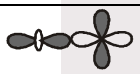
9. Match each of the diatomic molecules in **Column I** with its property/properties in **Column II**. **[JEE–2009, 8/160]**

	Column I		**Column II**
(A)	B_2	(p)	Paramagnetic
(B)	N_2	(q)	Undergoes oxidation
(C)	O_2^-	(r)	Undergoes reduction
(D)	O_2	(s)	Bond order ≥ 2
		(t)	Mixing of 's' and 'p' orbitals

10. Assuming that Hund's rule is violated, the bond order and magnetic nature of the diatomic molecule B_2 is :
(A) 1 and diamagnetic (B) 0 and diamagnetic **[JEE–2010, 5/163]**
(C) 1 and paramagnetic (D) 0 and paramagnetic

11. Assuming *2s-2p* mixing is **NOT** operative, the paramagnetic species among the following is : **[JEE(Advanced) 2014, 3/120]**
(A) Be_2 (B) B_2 (C) C_2 (D) N_2

12. Match the orbital overlap figures shown in List-I with the description given in List-II and select the correct answer using the code given below the lists. **[JEE(Advanced) 2014, 3/120]**

	List-I		**List-II**
P.		1.	*p–d* π antibonding
Q.		2.	*d–d* σ bonding
R.		3.	*p–d* π bonding
S.		4.	*d–d* σ antibonding

Code :

	P	Q	R	S		P	Q	R	S
(A)	2	1	3	4	(B)	4	3	1	2
(C)	2	3	1	4	(D)	4	1	3	2

13.* According to Molecular orbital Theory, **[JEE(Advanced) 2016, 4/124]**
(A) C_2^{2-} is expected to be diamagnetic
(B) O_2^{2+} is expected to have a longer bond length than O_2
(C) N_2^+ and N_2^- have the same bond order
(D) He_2^+ has the same energy as two isolated He atoms

PART - II : JEE (MAIN) / AIEEE PROBLEMS (PREVIOUS YEARS)

JEE(MAIN) ONLINE PROBLEMS

1. Increasing order of bond strength of O_2, O_2^-, O_2^{2-} and O_2^+ is : **[AIEEE-2002, 3/225]**
(1) $O_2^+ < O_2 < O_2^- < O_2^{2-}$ (2) $O_2 < O_2^+ < O_2^- < O_2^{2-}$
(3) $O_2^- < O_2^{2-} < O_2^+ < O_2$ (4) $O_2^{2-} < O_2^- < O_2 < O_2^+$

2. 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? **[AIEEE-2004, 3/225]**
(1) Bond length in NO^+ is greater than in NO (2) Bond length in NO is greater than in NO^+
(3) Bond length in NO^+ is equal to that in NO (4) Bond length is unpredictable

3. Which one of the following species is diamagnetic in nature ? **[AIEEE-2005, 1½/225]**
(1) He_2^+ (2) H_2 (3) H_2^+ (4) H_2^-.

4. Which of the following molecules/ions does not contain unpaired electrons? **[AIEEE-2006, 3/165]**
(1) O_2^{2-} (2) B_2 (3) N_2^+ (4) O_2

5. Which of the following species exhibits the diamagnetic behaviour? **[AIEEE-2007, 3/120]**
(1) O_2^{2-} (2) O_2^+ (3) O_2 (4) NO

6. In which of the following ionization processes, the bond order has increased and the magnetic behaviour has changed ? **[AIEEE-2007, 3/120]**
(1) $O_2 \longrightarrow O_2^+$ (2) $N_2 \longrightarrow N_2^+$ (3) $C_2 \longrightarrow C_2^+$ (4) $NO \longrightarrow NO^+$

7. Which one of the following pairs of species has the same bond order? **[AIEEE-2008, 3/105]**
(1) CN^- and CN^+ (2) O_2^- and CN^- (3) NO^+ and CN^+ (4) CN^- and NO^+

8. Using MO theory predict which of the following species has the shortest bond length ? **[AIEEE-2009, 4/144]**
(1) O_2^+ (2) O_2^- (3) O_2^{2-} (4) O_2^{2+}

9.* Which one of the following molecules is expected to exhibit diamagnetic behaviour ? **[JEE(Main)-2013, 4/120]**
(1) C_2 (2) N_2 (3) O_2 (4) S_2

10. In which of the following pairs of molecules/ions, both the species are not likely to exist ? **[JEE(Main)-2013, 4/120]**
(1) H_2^+, He_2^{2-} (2) H_2^-, He_2^{2-} (3) H_2^{2+}, He_2 (4) H_2^-, He_2^{2+}

11. Stability of the species Li_2, Li_2^- and Li_2^+ increases in the order of : **[JEE(Main)-2013, 4/120]**
(1) $Li_2 < Li_2^+ < Li_2^-$ (2) $Li_2^- < Li_2^+ < Li_2$ (3) $Li_2 < Li_2^- < Li_2^+$ (4) $Li_2^- < Li_2 < Li_2^+$

12. Which of the following species is not paramagnetic? **[JEE(Main)-2017, 4/120]**
(1) CO (2) O_2 (3) B_2 (4) NO

13. According to molecular orbital theory, which of the following will **not** be a viable molecule ? **[JEE(Main)-2018, 4/120]**
(1) H_2^- (2) H_2^{2-} (3) He_2^{2+} (4) He_2^+

JEE(MAIN) ONLINE PROBLEMS

1. Which of the following has unpaired electron(s) ? **[JEE(Main) 2014 Online (09-04-14), 4/120]**
(1) N_2 (2) O_2^- (3) N_2^{2+} (4) O_2^{2-}

2. The correct order of bond dissociation energy among N_2, O_2, O_2^- is shown in which of the following arrangements? **[JEE(Main) 2014 Online (11-04-14), 4/120]**
(1) $N_2 > O_2^- > O_2$ (2) $O_2^- > O_2 > N_2$ (3) $N_2 > O_2 > O_2^-$ (4) $O_2 > O_2^- > N_2$

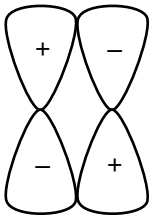
3. Which one of the following molecules is paramagnetic ? **[JEE(Main) 2014 Online (19-04-14), 4/120]**
(1) N_2 (2) NO (3) CO (4) O_3

4. After understanding the assertion and reason, choose the correct option.
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.
[JEE(Main) 2015 Online (10-04-15), 4/120]
(1) Assertion is correct, reason is incorrect.
(2) Assertion is incorrect, reason is correct.
(3) Assertion and reason are correct, but reason is not the correct explanation for the assertion.
(4) Assertion and reason are correct and reason is the correct and reason is the correct explanation for the assertion.

5. In the molecular orbital diagram for the molecular ion, N_2^+, the number of electrons in the σ_{2p} molecular orbital is : **[JEE(Main) 2018 Online (15-04-18), 4/120]**

(1) 0 (2) 2 (3) 3 (4) 1

6. Which of the following best describes the diagram below of a molecular orbital ? **[JEE(Main) 2018 Online (15-04-18), 4/120]**



(1) A non-bonding orbital (2) An antibonding σ orbital

(3) A bonding π orbital (4) An antibonding π orbital

7. According to molecular orbital theory, which of the following is true with respect to Li_2^+ and Li_2^- ? **[JEE(Main) 2019 Online (09-01-19), 4/120]**

(1) Li_2^+ is unstable and Li_2^- is stable (2) Li_2^+ is stable and Li_2^- is unstable

(3) Both are stable (4) Both are unstable

8. In which of the following processes, the bond order has increased and paramagnetic character has changed to diamagnetic? **[JEE(Main) 2019 Online (09-01-19), 4/120]**

(1) $NO \longrightarrow NO^+$ (2) $O_2 \longrightarrow O_2^{2-}$ (3) $O_2 \longrightarrow O_2^+$ (4) $N_2 \longrightarrow N_2^+$

Answers

EXERCISE - 1

PART – I

A-1. (a) 1 (b) 1/2 (c) 0 (d) 1 (e) 0 (f) 1

A-2. (a) B_2 (b) C_2 (c) O_2^{2+} (d) O_2 , (e) F_2 (f) N_2

A-3. 3

B-1. **Boron (B_2) :** B_2 is a good example of the energy level shift caused by the mixing of s and p orbitals. In the absence of mixing, the σ_g (2p) orbital is expected to be lower in energy than the π_u(2p) orbitals and the resulting molecule would be diamagnetic. However, mixing of the σ_g(2s) orbital with the σ_g(2p) orbital lowers the energy of the σ_g(2s) orbital and increases the energy of the σ_g(2p) orbital to a higher level than the π orbitals, giving the order of energies shown below. As a result, the last two electrons are unpaired in the degenerate (having the same energy) π orbitals, and the molecule is paramagnetic. $(\sigma 1s)^2$ $(\sigma^* 1s)^2$ $(\sigma 2s)^2$ $(\sigma^* 2s)^2$ $(\pi 2p^1_x = \pi 2p^1_y)$ $(\sigma p_z)^0$.

B-2. NO^+ and NO are derivative of N_2; so NO^+ bond order = 3 and NO bond order = 2.5; B.O. $\propto$ bond strength.

B-3. (ii) & (iv)

B-4. O–O bond length order is ii < i < iii

C-1. Weakest metallic bonding amongst the 3d-series elements $\rightarrow$ no unpaired electrons available for metallic bonding in case of zinc.

C-2. Be should have higher melting point as it contain 2 electrons for metallic bonding where as Li contain only one. Further more, size of Be is smaller than that of Li.

PART – II

A-1.	(C)	**A-2.**	(D)	**A-3.**	(C)	**A-4.**	(A)	**A-5.**	(D)
A-6.	(B)	**A-7.**	(C)	**B-1.**	(B)	**B-2.**	(A)	**B-3.**	(A)
B-4.	(C)	**B-5.**	(D)	**B-6.**	(D)	**C-1.**	(D)	**C-2.**	(D)

C-3. (D)

PART – III

1. (A – r) ; (B – p) ; (C – s) ; (D – q)

EXERCISE – 2

PART – I

1.	(A)	**2.**	(A)	**3.**	(C)	**4.**	(A)	**5.**	(D)
6.	(C)	**7.**	(A)	**8.**	(D)	**9.**	(C)	**10.**	(D)
11.	(A)								

PART – II

1.	4 (a, b, d, g)	**2.**	6 (a, b, c, d, e, f)
3.	4 (ii, iv, vi, vii)	**4.**	9 (a, b, c, d, e, f, g, j, k)

PART – III

1.	(ABC)	**2.**	(ABC)	**3.**	(BD)	**4.**	(ABC)	**5.**	(AC)
6.	(BC)	**7.**	(ABD)						

PART – IV

1.	(D)	**2.**	(D)	**3.**	(B)	**4.**	(C)	**5.**	(A)
6.	(D)	**7.**	(C)	**8.**	(D)	**9.**	(B)	**10.**	(C)
11.	(D)								

EXERCISE – 3

PART – I

1. Molecular orbital electronic configuration of O_2 is as follows (Z is taken as molecular axis).

$\sigma_{1s^2}\ \sigma^*_{1s^2}\ \sigma_{2s^2}\ \sigma^*_{2s^2}\ \sigma_{2p_z^2}\ \pi_{2p_x^2} = \pi_{2p_y^2}\ \pi^*_{2p_x^1} = \pi^*_{2p_y^1}$.

Bond order = $\frac{10-6}{2}$ = 2.

As it contains two unpaired electrons in bonding π molecular orbitals O_2 is paramagnetic.

So, Magnetic moment = $\sqrt{n\ \ (n+2)}$ = $\sqrt{2\ \ (2+2)}$ = 2.83 B.M.

2. (C) **3.** (B)

4. The electronic configuration of O_2 will be:

$O_2 = \sigma1s^2\ \sigma^*1s^2\ \sigma2s^2\ \sigma^*2s^2\ \sigma2p^2_z\ \pi2p^2_x = \pi2p^2_y\ \pi^*2p^1_x = \pi^*2p^1_y$

Now bond order = $\frac{N_b - N_a}{2}$

Where, N_b = Number of electrons in bonding orbitals

N_a = Number of electrons in antibonding orbitals

bond order = $\frac{10-6}{2}$ = 2

Similarly electronic configuration of O_2^- (in KO_2) will be

$\sigma 1s^2\ \sigma^*1s^2\ \sigma 2s^2\ \sigma^*2s^2\ \sigma 2p^2_z\ \pi 2p^2_x = \pi 2p^2_y\ \pi^*2p^2_x = \pi^*2p^1_y$

Bond order = $\frac{10-7}{2} = \frac{3}{2}$ = 1.5 In $O_2[AsF_4]^-$, O_2 is O_2^+ .

The electronic configuration of O_2^+ will be

$\sigma 1s^2\ \sigma^*1s^2\ \sigma 2s^2\ \sigma^*2s^2\ \sigma 2p^2_z\ \pi^2 p^2_x, = \pi 2p^2_y\ \pi^*2p^1_x$

bond order = $\frac{10-5}{2} = 2.5$

Hence bond length order will be $O^+_2 < O_2 < O^-_2$ because Bond order $\propto \frac{1}{\text{Bond length}}$.

5. (A) **6.** (D) **7.** (C) **8.** (A)

9. (A) - p, q, r, t ; (B) - q, r, s, t ; (C) - p, q, r ; (D) - p, q, r, s

10. (A) **11.** (C) **12.** (C) **13.*** (AC)

PART – II

JEE(MAIN) OFFLINE PROBLEMS

1. (4) **2.** (2) **3.** (2) **4.** (1) **5.** (1)

6. (4) **7.** (4) **8.** (4) **9.*** (1, 2) **10.** (3)

11. (2) **12.** (1) **13.** (2)

JEE(MAIN) ONLINE PROBLEMS

1. (2) **2.** (3) **3.** (2) **4.** (1) **5.** (4)

6. (4) **7.** (3) **8.** (1)