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Molecular Orbital Theory

Chemistry Affinity

Conceptual, Real World, Happy Learning

Which among the following process is /are associated with increasing bond order but no change in diamagnetic /paramagnetic bebaviour?

(i) $N_2 \longrightarrow N_2^+ + e$ (ii) $O_2 \longrightarrow O_2^+ + e$ (iii) $O_2 + e \longrightarrow O_2^-$

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(a) (ii) only

(b) (i) and (ii)

(c) (ii) and (iii)

(d) (iii) only

Nitrogen atoms: 5 valence electrons
N_2 molecule: 10 valence electrons

$\sigma_{2s}^2\ \sigma_{2s}^{*2}\ \pi_{2p_x}^2\ \pi_{2p_y}^2\ \sigma_{p_z}^2 \Rightarrow N_2 \Rightarrow$ Diamagnetic

$\sigma_{2s}^2\ \sigma_{2s}^{*2}\ \pi_{2p_x}^2\ \pi_{2p_y}^2\ \sigma_{p_z}^1 \Rightarrow N_2^+ \Rightarrow$ Paramagnetic

Bond order (BO) = $\dfrac{\text{no of bonding electrons} - \text{no of antibonding electrons}}{2}$

$N_2 : BO = \dfrac{8-2}{2} = 3$

$N_2^+ : BO = \dfrac{7-2}{2} = 2.5$

Oxygen atoms: 6 valence electrons
O_2 molecule: 12 valence electrons

$\sigma_{2s}^2\ \sigma_{2s}^{*2}\ \sigma_{2p_x}^2\ \pi_{2p_y}^2\ \pi_{2p_z}^2\ \pi_{2p_y}^{*1}\ \pi_{2p_z}^{*1} : O_2$ $\quad BO = \frac{8-4}{2} = 2$

Paramagnetic

$\sigma_{2s}^2\ \sigma_{2s}^{*2}\ \sigma_{2p_x}^2\ \pi_{2p_y}^2\ \pi_{2p_z}^2\ \pi_{2p_y}^{*1}\ \pi_{2p_z}^{*} : O_2^+$ $\quad BO = \frac{8-3}{2} = 2.5$

Paramagnetic

$\sigma_{2s}^2\ \sigma_{2s}^{*2}\ \sigma_{2p_x}^2\ \pi_{2p_y}^2\ \pi_{2p_z}^2\ \pi_{2p_y}^{*2}\ \pi_{2p_z}^{*1} = O_2^-$ $\quad BO = \frac{8-5}{2} = 1.5$

Paramagnetic

Bond order increases but paramagnetic behavior remain same

(ii) $O_2 \longrightarrow O_2^+ + e$

Correct option (II) only

What is bond order? Describe the Bond order determination of O_2 molecule and the significance of LCOA theory to explain the magnetic properties of Oxygen.

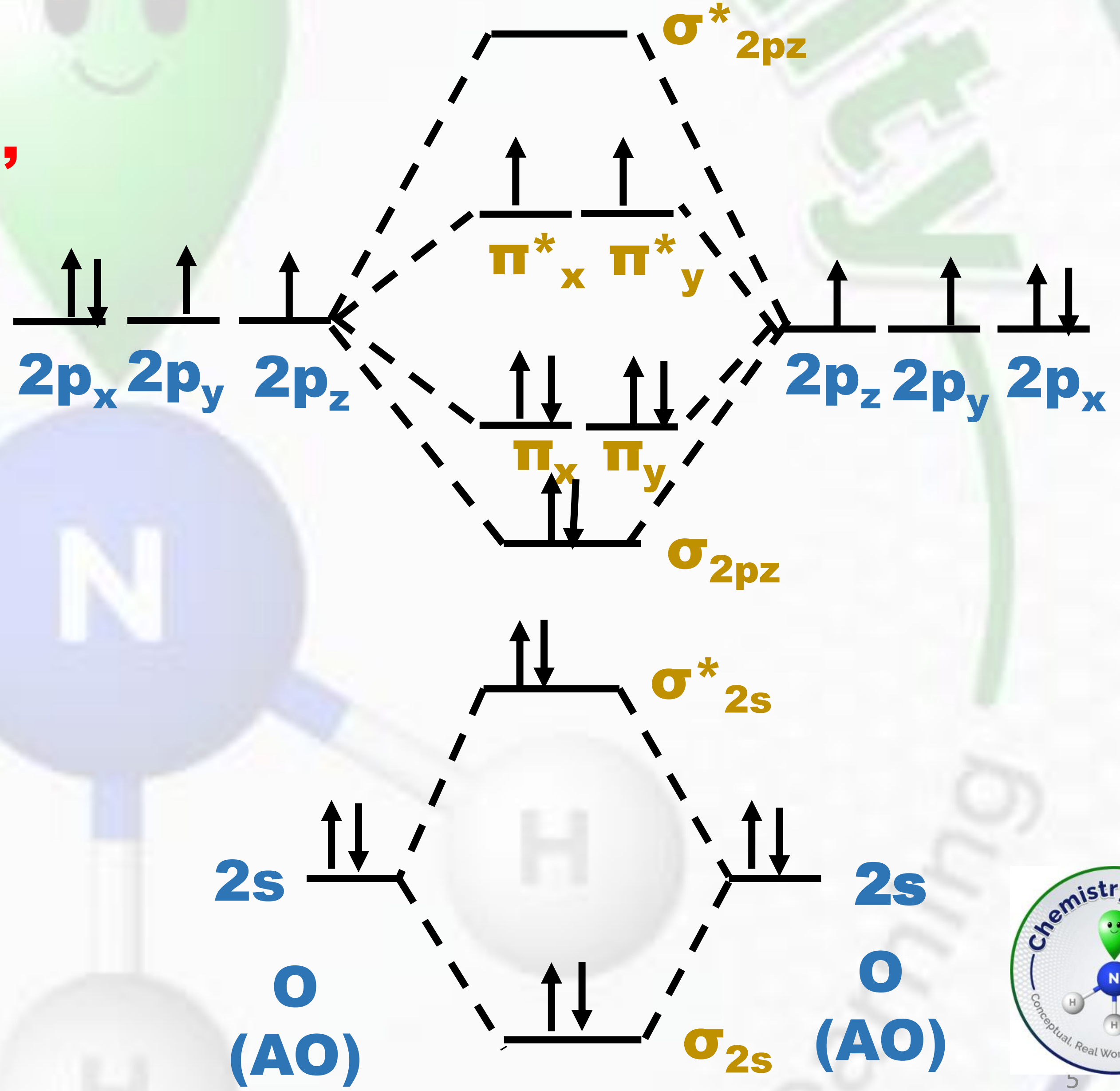
The number of bonds between a pair of atoms is called the bond order

Bond order (BO) = $\frac{no\ of\ bonding\ electrons - no\ of\ antibonding\ electrons}{2}$

O_2: σ_{2s}^2, $\sigma^*_{2s}{}^2$, σ_{2pz}^2, π_{2px}^2 π_{2py}^2, $\pi^*_{2px}{}^1$ $\pi^*_{2py}{}^1$

Bond order = (8-4)/2 = 2

Two unpaired electrons, O_2 is paramagnetic



Carbon monoxide has ten bonding electrons and four antibonding electrons.
Therefore, it has a bond order of
(a) 3
(b) 7
(c) 1
(d) 5/2
(e) 2

Bond order (BO) = $\frac{no\ of\ bonding\ electrons\ - no\ of\ antibonding\ electrons}{2}$

Bond order (BO) = $\frac{10-4}{2}$

Bond order (BO) = 3

Correct option (a) 3

Which of the following is the correct electron configuration for C_2?

(a) $\sigma_{1s}^2\ \sigma_{2s}^2\ \pi_{2py}^2\ \sigma^*_{1s}{}^2\ \sigma^*_{2s}{}^2\ \pi^*_{2py}{}^2$

(b) $\sigma_{1s}^2\ \sigma^*_{1s}{}^2\ \sigma_{2s}^2\ \sigma^*_{2s}{}^2\ \pi_{2py}^2\ \pi^*_{2pz}{}^1\ \sigma_{2p}^1$

(c) $\sigma_{1s}^2\ \sigma^*_{1s}{}^2\ \sigma_{2s}^2\ \sigma^*_{2s}{}^2\ \pi_{2py}^2\ \pi_{2pz}^2$

(d) $\sigma_{1s}^2\ \sigma^*_{1s}{}^2\ \sigma_{2s}^2\ \sigma^*_{2s}{}^2\ \pi_{2py}^1\ \pi_{2pz}^1$

(e) $\sigma_{1s}^2\ \sigma^*_{1s}{}^2\ \sigma_{2s}^2\ \sigma^*_{2s}{}^2\ \pi_{2py}^1\ \pi^*_{2py}{}^1\ \pi_{2pz}^1\ \pi^*_{2pz}{}^1$

C_2: σ_{1s}^2, $\sigma^*_{1s}{}^2$, σ_{2s}^2, $\sigma^*_{2s}{}^2$, π_{2px}^2 π_{2py}^2

Correct option (c)

What is the correct electron configuration for the molecular ion, B_2^+?

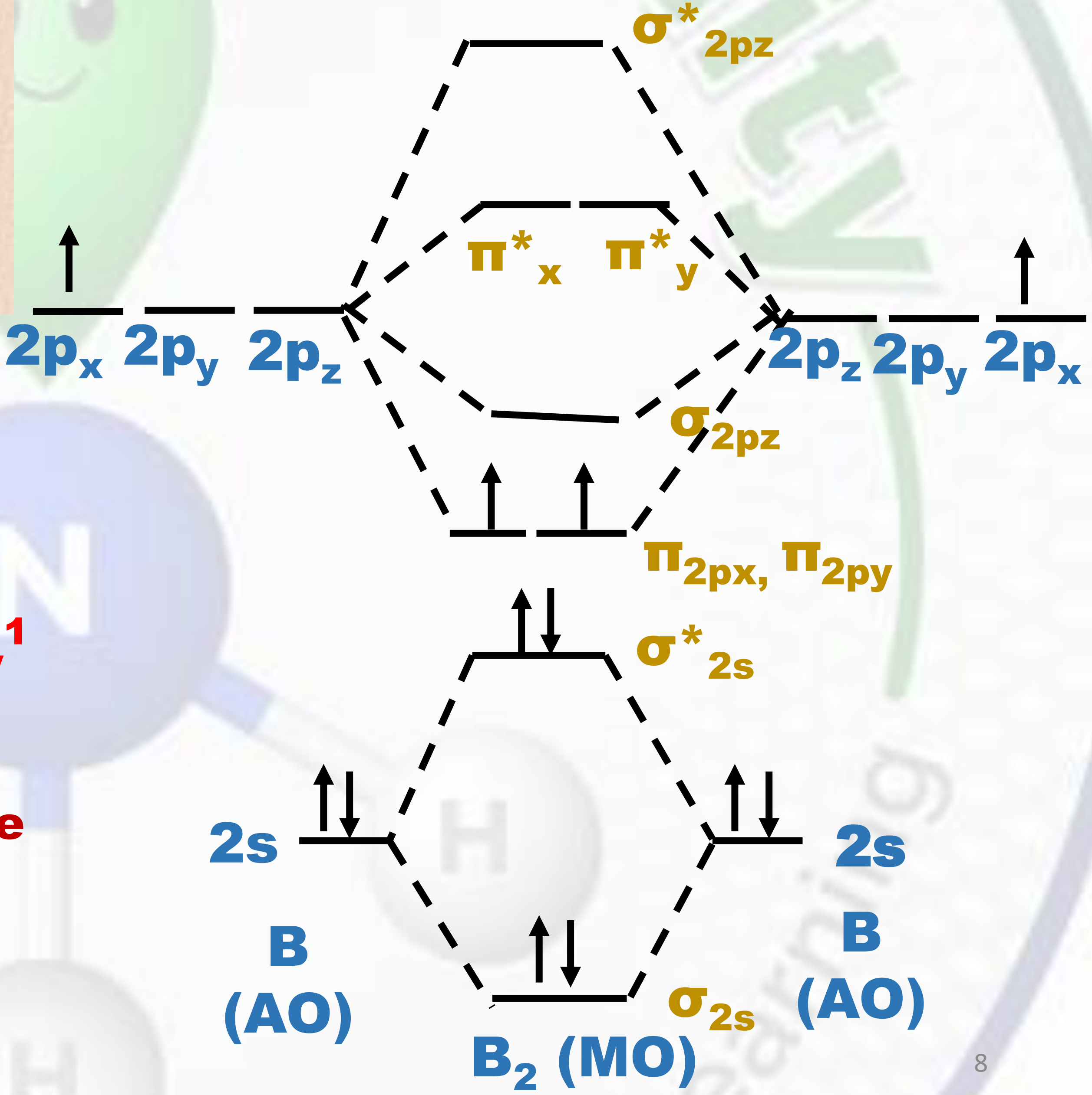
(a) $\sigma_{1s}^2\ \sigma^*_{1s}{}^2\ \sigma_{2s}^2\ \sigma^*_{2s}{}^2\ \sigma_{2p}^2$

(b) $\sigma_{1s}^2\ \sigma^*_{1s}{}^2\ \sigma_{2s}^2\ \sigma^*_{2s}{}^2\ \pi_{2py}^2$

(c) $\sigma_{1s}^2\ \sigma^*_{1s}{}^2\ \sigma_{2s}^2\ \sigma^*_{2s}{}^2\ \pi_{2py}^2\ \pi_{2pz}^1$

(d) $\sigma_{1s}^2\ \sigma^*_{1s}{}^2\ \sigma_{2s}^2\ \sigma^*_{2s}{}^2\ \sigma_{2p}^1\ \pi_{2py}^1$

(e) none of the above.



B: $1s^2, 2s^2, 2p^1$

B_2: $\sigma_{1s}^2, \sigma^*_{1s}{}^2, \sigma_{2s}^2, \sigma^*_{2s}{}^2, \pi_{2px}^1\ \pi_{2py}^1$

Correct option (e) None of the above

The number of unpaired electrons in B_2 molecule is

(a) 1, (b) 2, © 3, (d) 4

B_2: $\sigma_{1s}^2, \sigma^*_{1s}^2, \sigma_{2s}^2, \sigma^*_{2s}^2, \pi_{2px}^1\ \pi_{2py}^1$

Number of unpaired electrons are 2

Correct option (b) 2

For the molecular ion N_2^+.The number of electrons in the σ_{2p} molecular orbital is (a) o, (b) 1, © 2, (d) 3

$\sigma_{2s}^2 \sigma_{2s}^{*2} \pi_{2p_x}^2 \pi_{2p_y}^2 \sigma_{p_z}^2 \Rightarrow N_2 \Rightarrow$ Diamagnetic

$\sigma_{2s}^2 \sigma_{2s}^{*2} \pi_{2p_x}^2 \pi_{2p_y}^2 \sigma_{p_z}^1 \Rightarrow N_2^+ \Rightarrow$ Paramagnetic

Correct option (b) 1

What is the bond order in O_2^+. (a) 3.5, (b) 2, © 1.5, (d) 2.5

$\sigma_{2s}^{2}\,\sigma_{2s}^{*2}\,\sigma_{2p_x}^{2}\,\pi_{2p_y}^{2}\,\pi_{2p_z}^{2}\,\pi_{2p_y}^{*1}\,\pi_{2p_z}^{*1}$: O_2 $\quad BO = \frac{8-4}{2} = 2$

$\sigma_{2s}^{2}\,\sigma_{2s}^{*2}\,\sigma_{2p_x}^{2}\,\pi_{2p_y}^{2}\,\pi_{2p_z}^{2}\,\pi_{2p_y}^{*1}\,\pi_{2p_z}^{*}$ = O_2^+ $\quad BO = \frac{8-3}{2} = 2.5$

Correct option (d) 2.5

Antibonding molecular orbitals are produced by

(a) Constructive interaction of atomic orbitals
(b) Destructive interaction of atomic orbitals
(c) The overlap of the atomic orbitals of two negative ions
(d) All of these

Correct option (b) Destructive interaction of atomic orbitals

According to molecular orbital theory, the species among the following that does not exist is : (a) O_2^- (b) Be_2, (c) He_2^-, (d) He_2^+

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(a) $\sigma_{2s}^2\ \sigma_{2s}^{*2}\ \sigma_{2p_x}^2\ \pi_{2p_y}^2\ \pi_{2p_z}^2\ \pi_{2p_y}^{*2}\ \pi_{2p_z}^{*1} = O_2^-$ $BO = \frac{8-5}{2} = 1.5$

(b) Be : $1s^2\ 2s^2$

$\sigma_{1s}^2\ \sigma_{1s}^{*2}\ \sigma_{2s}^2\ \sigma_{2s}^{*2}$ $BO = \frac{4-4}{2} = 0$

Correct option (b) Be_2

(c) He : $1s^2$

He_2^- : $\sigma_{1s}^2\ \sigma_{1s}^{*2}\ \sigma_{2s}^1$ $BO = \frac{3-2}{2} = 0.5$

(d) He_2^+ : $\sigma_{1s}^2\ \sigma_{1s}^{*1}$ $BO = \frac{2-1}{2} = 0.5$

The linear combination of atomic orbitals to form molecular orbitals takes place only when the combining orbitals are

(A) have the same energy (B) have the minimum overlap (c) have same symmetry about the molecular axis (D) have different symmetry about the molecular axis

(i) A, B and C, (II) A and C only (iii) B and D only , (iv) B, C and D only

Correct option (II) A and C only

When two atomic orbitals combine, they form

(A) One molecular orbital (B) Two molecular orbital (c) Three molecular orbitals (D) Four molecular orbitals

Correct option (B) Two molecular orbitals

Which of the following is least stable

(A) O_2 (B) O_2^{2-} (c) O_2^{+1} (D) O_2^{-1}

(A) $\sigma_{2s}^2\ \sigma^*{}_{2s}^2\ \sigma_{2p_x}^2\ \pi_{2p_y}^2\ \pi_{2p_z}^2\ \pi^*{}_{2p_y}^1\ \pi^*{}_{2p_z}^1$: O_2 $BO = \frac{8-4}{2} = 2$

(B) $\sigma_{2s}^2\ \sigma^*{}_{2s}^2\ \sigma_{2p_x}^2\ \pi_{2p_y}^2\ \pi_{2p_z}^2\ \pi^*{}_{2p_y}^2\ \pi^*{}_{2p_z}^2$: O_2^{2-} $BO = \frac{8-6}{2} = 1$

(c) $\sigma_{2s}^2\ \sigma^*{}_{2s}^2\ \sigma_{2p_x}^2\ \pi_{2p_y}^2\ \pi_{2p_z}^2\ \pi^*{}_{2p_y}^1\ \pi^*{}_{2p_z}$: O_2^+ $BO = \frac{8-3}{2} = 2.5$

(d) $\sigma_{2s}^2\ \sigma^*{}_{2s}^2\ \sigma_{2p_x}^2\ \pi_{2p_y}^2\ \pi_{2p_z}^2\ \pi^*{}_{2p_y}^2\ \pi^*{}_{2p_y}^1$ = O_2^{-1} $BO = \frac{8-5}{2} = 1.5$

Lowest bond order means least stable because it needs less energy to break the bond. Therefore, O_2^{2-} is least stable. Correct option (B)

All the best