

Chapter-6

INNOVATIVE METHOD FOR THE PREDICTION OF THE MAGNETIC BEHAVIOUR AND BOND ORDER OF DIATOMIC SPECIES WITHOUT MOLECULAR ORBITAL THEORY

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In chapter 4, formulae-based mnemonics have been discussed to predict the bond order of homo and heteronuclear diatomic species without drawing their electronic configurations based on molecular orbital theory (M.O.T.). In chapter 5, the prediction of bond order of oxide-based acid radicals has been discussed without drawing Lewis structures in a time economic way. In this chapter 6, magnetic properties of diatomic species having the total number of electrons (1-20), have been predicted without drawing electronic configuration by using molecular orbital theory. Here, three (03) time economic innovative mnemonics have been discussed by including three (03) formulae to predict the magnetic behavior of diatomic species without using M.O.T. Conventionally, magnetic properties of diatomic species, predicted from the Molecular Orbital Theory by counting the number of unpaired electrons present in the bonding molecular orbitals (BMOs) or antibonding molecular orbitals (ABMOs) of diatomic species. If in the electronic configuration, diatomic species, contain unpaired or paired electrons in its bonding molecular orbitals (BMOs) or antibonding molecular orbitals (ABMOs), then it will be paramagnetic or diamagnetic, respectively. **In this chapter 6, adequate examples on the prediction of bond order of homo and heteronuclear diatomic molecules or ions having the total number of electrons fall in the range (1-20) without molecular orbital theory (discussed in chapter 4) have been explored also in the tabulated form.**

Molecular Orbital Theory (M.O.T.) was first proposed by Friedrich Hund and Robert Mulliken in 1933^{1,2}. The present chapter 6, involves three (03) formulae by just manipulating the number of unpaired electrons (n), using mod function and by means of these n values, students can easily stumble upon the magnetic moment values in Bohr-Magneton (B.M.) using spin only formula $\mu_s = \sqrt{n(n+2)}$ B.M., where, B.M. = Bohr Magneton = unit of magnetic moment and n = number of unpaired electrons^{3,4,5,6}.

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2. George G. Hall, "The Lennard-Jones Paper of 1929 and the foundations of Molecular Orbital Theory", *Advances in Quantum Chemistry* 22 (1991): 1-6, doi:10.1016/S0065-3276(08)60361-5.

3.A.Das, "Bond-order and Magnetic Behavior of Diatomic Species without Molecular Orbital Theory", *World Journal of Chemical Education* 5 (June 2017):128-131, doi: 10.12691/wjce-5-4-2, <http://pubs.sciepub.com/wjce/5/4/2/>.

4. A. Das, "A Review of Time Economic Innovative Mnemonics In Chemical Education". *International Journal of Physics & Chemistry Education* 10 (June 2018):27-40, doi: 10.12973/ijpce/81589, <http://www.ijpce.org/A-Review-of-Time-Economic-Innovative-Mnemonics-in-Chemical-Education,81589,0,2.html>.

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6. A. Das, "Innovative Mnemonics Make Chemical Education Time Economic – A Pedagogical Review Article", *World Journal of Chemical Education* 6 (Sept 2018):154-174, doi:10.12691/wjce-6-4-2, <http://pubs.sciepub.com/wjce/6/4/2/index.html>.

METHODOLOGY

A. Conventional method for prediction of magnetic properties of diatomic species with molecular orbital theory

Increasing energetic order of different molecular orbitals for number of electrons ≤ 14

$$\sigma_{1s} < \sigma_{1s}^* < \sigma_{2s} < \sigma_{2s}^* < \pi_{2px} = \pi_{2py} < \sigma_{2pz} < \pi_{2px}^* = \pi_{2py}^* < \sigma_{2pz}^*$$

Increasing energetic order of different molecular orbitals for number of electrons > 14

$$\sigma_{1s} < \sigma_{1s}^* < \sigma_{2s} < \sigma_{2s}^* < \sigma_{2pz} < \pi_{2px} = \pi_{2py} < \pi_{2px}^* = \pi_{2py}^* < \sigma_{2pz}^*$$

In this energetic order, there is five bonding molecular orbitals (BMOs), σ_{1s} , σ_{2s} , π_{2px} , π_{2py} , σ_{2pz} and five anti bonding molecular orbitals (ABMOs), σ_{1s}^* , σ_{2s}^* , π_{2px}^* , π_{2py}^* , σ_{2pz}^* . Magnetic properties of diatomic species predicted from the electronic configuration of diatomic species by counting the number of unpaired electrons present in the bonding molecular orbitals (BMOs) or anti bonding molecular orbitals (ABMOs) of diatomic species. If the diatomic species contain unpaired or paired electrons in its bonding molecular orbitals (BMOs) or anti bonding molecular orbitals (ABMOs), then it will be paramagnetic or diamagnetic respectively.

B. Innovative method for the prediction of magnetic properties of diatomic species without molecular orbital theory

First, classify the molecules or ions in **three (03) sets** depending on the total number of electrons present in them as follows:

Set-1: Molecules or ions having (1-3)e's, (3-5)e's, (5-7)e's, (7-10)e's, (13-16)e's

Set-2: Molecules or ions having (10-13)e's and (16-19)e's

Set-3: Molecules or ions having 20 e's

Then for a different set, we must use three different formulae to calculate the number of unpaired electrons and thus magnetic moment (μ_s) in B.M. can be evaluated in the following way:

i)F-1(For Set-1) - for the determination of the number of unpaired electrons (n) of molecules or ions having the total number of electrons (1-3), (3-5), (5-7), (7-10) and (13-16)e's:

$$\text{In this case, the number of unpaired electrons } n = [I (ND - \text{total e's}) I]$$

Here, ND = next digit (digit next to minimum digit) and 'I' indicates mod function.

Ex. Molecules or ions having (1-3)e's, in this case, ND = 2 because here minimum digit is 1.

For the molecules or ions containing (3-5)e⁻s, (5-7)e⁻s, (7-10)e⁻s, and (13-16)e⁻s, the ND value will be 4, 6, 8 and 14 respectively. Hence, the value of $n = [I (4\text{-total } e^-) I]$; $[I (6\text{- total } e^-) I]$ $[I (8\text{- total } e^-) I]$ and $[I (14\text{- total } e^-) I]$ respectively.

ii) F-2 (For Set-2) - for the determination of number of unpaired electrons (n) of molecules or ions having total number of electrons (10-13) and (16-19):

In this case, the number of unpaired electrons $n = [I (PD - \text{total } e^-) I]$

Here, PD = Penultimate digit (digit before last electron digit).

For the molecules or ions containing (10-13) and (16-19)e⁻s, the PD value will be 12 and 18 respectively. Hence, the value of $n = [I (12 - \text{total } e^-) I]$ and $[I (18 - \text{total } e^-) I]$ respectively.

iii) F-3 (For Set-3) - for the determination of number of unpaired electrons (n) of molecules or ions having total number of electrons 20:

In this case, the number of unpaired electrons $n = [(20 - \text{total } e^-)]$

RESULTS AND DISCUSSION

A. Prediction of magnetic properties by conventional method using M.O.T.:

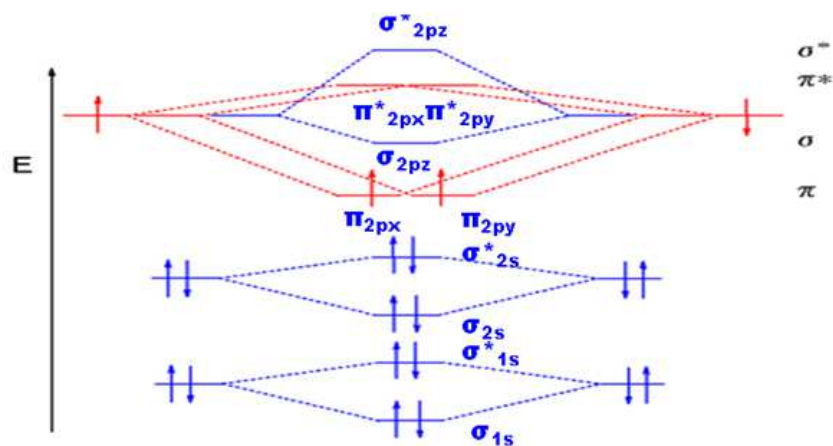
By using conventional method magnetic properties of molecules or ions should be predicted in the following way:

Ex. H₂ (number of electrons < 14) : Electronic configuration (E.C.) with MOT σ_{1s}^2 , unpaired electrons (n) = 0, diamagnetic in nature ; **H₂⁺**: E.C. is σ_{1s}^1 , unpaired electron (n) = 1, paramagnetic in nature; **H₂⁻**: E.C. is $\sigma_{1s}^2, \sigma_{1s}^{*1}$, unpaired electron (n) = 1, paramagnetic in nature.

He₂: E.C. is $\sigma_{1s}^2, \sigma_{1s}^{*2}$, unpaired electrons (n) = 0, diamagnetic in nature; **He₂⁺** : E.C. is $\sigma_{1s}^2, \sigma_{1s}^{*1}$, unpaired electron (n) = 1, paramagnetic in nature.

Li₂: E.C. is $\sigma_{1s}^2, \sigma_{1s}^{*2}, \sigma_{2s}^2$, unpaired electron (n) = 0, diamagnetic in nature; **Be₂**: E.C. is $\sigma_{1s}^2, \sigma_{1s}^{*2}, \sigma_{2s}^2, \sigma_{2s}^{*2}$, unpaired electron (n) = 0, diamagnetic in nature; **B₂**: E.C. is $\sigma_{1s}^2, \sigma_{1s}^{*2}, \sigma_{2s}^2, \sigma_{2s}^{*2}, \pi_{2px}^1, \pi_{2py}^1$ (**Fig.4.22**), unpaired electrons (n) = 2, paramagnetic in nature; **C₂**: E.C. is $\sigma_{1s}^2, \sigma_{1s}^{*2}, \sigma_{2s}^2, \sigma_{2s}^{*2}, \pi_{2px}^2, \pi_{2py}^2$, unpaired electron (n) = 0, diamagnetic in nature.

Molecular Orbital Diagram of B₂ having electrons < 14



$$\text{Bond order of B}_2 = \frac{\text{without star orbital (BMO)} - \text{with star orbital (ABMO)}}{2} = \frac{6-4}{2}$$

Fig.4.22: Molecular orbital diagram of B₂

N₂: E.C. is $\sigma_{1s}^2, \sigma_{1s}^{*2}, \sigma_{2s}^2, \sigma_{2s}^{*2}, \pi_{2px}^2, \pi_{2py}^2, \sigma_{2pz}^2$, unpaired electron (n) = 0, diamagnetic in nature; **N₂⁺**: E.C. is $\sigma_{1s}^2, \sigma_{1s}^{*2}, \sigma_{2s}^2, \sigma_{2s}^{*2}, \pi_{2px}^2, \pi_{2py}^2, \sigma_{2pz}^1$, unpaired electron (n) = 1, paramagnetic in nature; **N₂⁻**: E.C. is $\sigma_{1s}^2, \sigma_{1s}^{*2}, \sigma_{2s}^2, \sigma_{2s}^{*2}, \pi_{2px}^2, \pi_{2py}^2, \sigma_{2pz}^2, \pi_{2px}^{*1}$, unpaired electron (n) = 1, paramagnetic in nature; **N₂²⁻**: E.C. is $\sigma_{1s}^2, \sigma_{1s}^{*2}, \sigma_{2s}^2, \sigma_{2s}^{*2}, \pi_{2px}^2, \pi_{2py}^2, \sigma_{2pz}^2, \pi_{2px}^{*1}, \pi_{2py}^{*1}$, unpaired electrons (n) = 2, paramagnetic in nature.

O₂ (number of electrons > 14): E.C. of O₂ is $\sigma_{1s}^2, \sigma_{1s}^{*2}, \sigma_{2s}^2, \sigma_{2s}^{*2}, \sigma_{2pz}^2, \pi_{2px}^2, \pi_{2py}^2, \pi_{2px}^{*1}, \pi_{2py}^{*1}$ (**Fig.4.23**), unpaired electrons (n) = 2, paramagnetic in nature; **O₂⁺**: E.C. is $\sigma_{1s}^2, \sigma_{1s}^{*2}, \sigma_{2s}^2, \sigma_{2s}^{*2}, \sigma_{2pz}^2, \pi_{2px}^2, \pi_{2py}^2, \pi_{2px}^{*1}$, unpaired electron (n) = 1, paramagnetic in nature; **O₂⁻**: E.C. is $\sigma_{1s}^2, \sigma_{1s}^{*2}, \sigma_{2s}^2, \sigma_{2s}^{*2}, \sigma_{2pz}^2, \pi_{2px}^2, \pi_{2py}^2, \pi_{2px}^{*2}, \pi_{2py}^{*1}$, unpaired electron (n) = 1, paramagnetic in nature; **O₂²⁻**: E.C. is $\sigma_{1s}^2, \sigma_{1s}^{*2}, \sigma_{2s}^2, \sigma_{2s}^{*2}, \sigma_{2pz}^2, \pi_{2px}^2, \pi_{2py}^2, \pi_{2px}^{*2}, \pi_{2py}^{*2}$, unpaired electron (n) = 0, diamagnetic in nature.

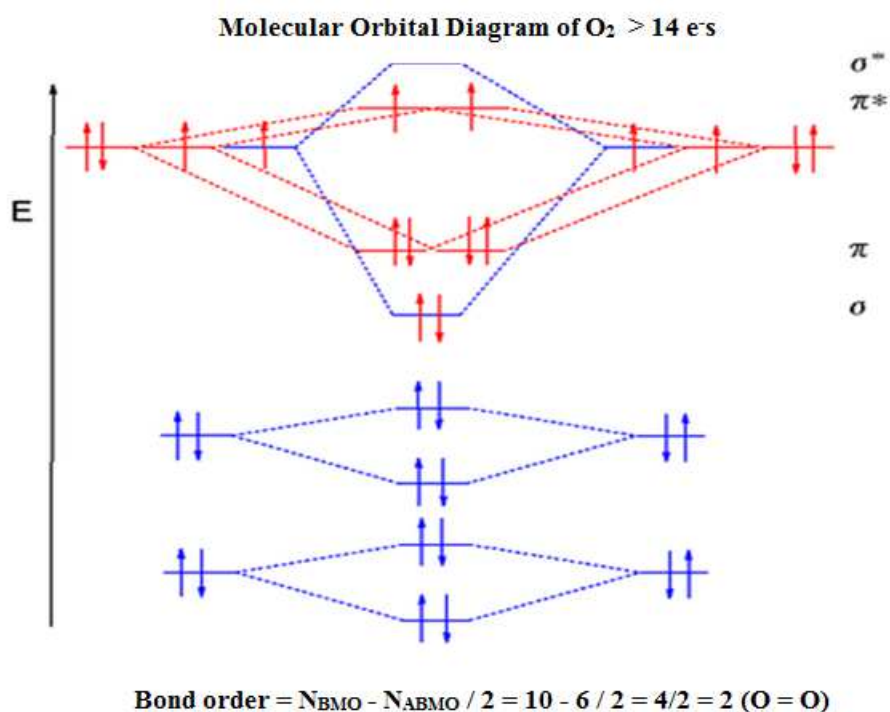


Fig.4.23: Molecular orbital diagram of O₂

F₂: E.C. is $\sigma_{1s}^2, \sigma_{1s}^{*2}, \sigma_{2s}^2, \sigma_{2s}^{*2}, \sigma_{2pz}^2, \pi_{2px}^2, \pi_{2py}^2, \pi_{2px}^{*2}, \pi_{2py}^{*2}$, unpaired electron (n) = 0, diamagnetic in nature.

Ne₂: E.C. is $\sigma_{1s}^2, \sigma_{1s}^{*2}, \sigma_{2s}^2, \sigma_{2s}^{*2}, \sigma_{2pz}^2, \pi_{2px}^2, \pi_{2py}^2, \pi_{2px}^{*2}, \pi_{2py}^{*2}, \sigma_{2pz}^{*2}$, unpaired electron (n) = 0, diamagnetic in nature.

CN (number of electrons < 14): E.C. is $\sigma_{1s}^2, \sigma_{1s}^{*2}, \sigma_{2s}^2, \sigma_{2s}^{*2}, \pi_{2px}^2, \pi_{2py}^2, \sigma_{2pz}^1$, unpaired electron (n) = 1, paramagnetic in nature; **CN⁺:** E.C. is $\sigma_{1s}^2, \sigma_{1s}^{*2}, \sigma_{2s}^2, \sigma_{2s}^{*2}, \pi_{2px}^2, \pi_{2py}^2, \sigma_{2pz}^2$, unpaired electron (n) = 0, diamagnetic in nature.

NO (number of electrons > 14): E.C. is $\sigma_{1s}^2, \sigma_{1s}^{*2}, \sigma_{2s}^2, \sigma_{2s}^{*2}, \sigma_{2pz}^2, \pi_{2px}^2, \pi_{2py}^2, \pi_{2px}^{*1}$, unpaired electron (n) = 1, paramagnetic in nature; **NO⁺:** E.C. is $\sigma_{1s}^2, \sigma_{1s}^{*2}, \sigma_{2s}^2, \sigma_{2s}^{*2}, \sigma_{2pz}^2, \pi_{2px}^2, \pi_{2py}^2$, unpaired electron (n) = 0, diamagnetic in nature.

B. Prediction of magnetic properties by innovative method without M.O.T.:

The present study involves three (03) new formulae by just manipulating the number of unpaired electrons (n) using mod function (based on Applied Mathematics) and from these 'n' values, the magnetic moment values in Bohr-Magneton, can be calculated by using spin only formula, $\mu_s = \sqrt{n(n+2)}$ B.M., where B.M. = Bohr Magneton = Unit of Magnetic Moment, n = number of unpaired electrons.

First, classify the molecules or ions depending on the total number of electrons present in them in the following three (03) sets:

Set-1: Molecules or ions having (1-3)e-s, (3-5)e-s, (5-7)e-s, (7-10)e-s, (13-16)e-s

Set-2: Molecules or ions having (10-13)e-s and (16-19)e-s

Set-3: Molecules or ions having 20e-s

For the different set, there are three (03) different formulae to calculate the number of unpaired electrons (n), which have been presented in **Table 5.5**.

The magnetic moment values (μ_s), in B.M., can be evaluated from the number of unpaired electrons (n) in the following way:

F-1(For Set-1) - for the determination of number of unpaired electrons (n) of molecules or ions having the total number of electrons (1-3), (3-5), (5-7), (7-10) and (13-16)e-s: In this case, the number of unpaired electrons $n = [I (ND - \text{total e-s}) I]$ Here, ND = next digit i.e. digit next to minimum digit and 'I' indicates mod function.

For molecules or ions having (1-3)e-s, ND = 2, because here, the minimum digit is 1.

Ex.a. In He_2^+ (3e-s), the total number of electrons will be 3, ND = 2, hence, unpaired electron $n = I (ND - \text{total e-s}) I = I (2-3) I = 1$, hence, magnetic moment, $\mu_s = \sqrt{n(n+2)} \text{ B.M.} = \sqrt{1(1+2)} \text{ B.M.} = \sqrt{3} \text{ B.M.} = 1.73 \text{ B.M.}$

For molecules or ions containing (3-5)e-s, (5-7)e-s, (7-10)e-s, and (13-16)e-s the ND value will be 4, 6, 8 and 14 respectively. Hence, the value of $n = [I (4-\text{total e-s}) I]$; $[I (6-\text{total e-s}) I]$; $[I (8-\text{total e-s}) I]$ and $[I (14-\text{total e-s}) I]$ respectively.

F-2(For Set-2) - for the determination of number of unpaired electrons (n) of molecules or ions having total number of electrons (10-13) and (16-19): In this case, the number of unpaired electrons $n = [I (PD - \text{total e-s}) I]$, where, PD = Penultimate digit (i.e. digit before last electron).

Ex.b. In C_2^- (13e-s), the total number of electrons will be 13, PD = 12, Hence, unpaired electron $n = I (12 - \text{total e-s}) I = I (12-13) I = 1$ and magnetic moment, $\mu_s = \sqrt{n(n+2)} \text{ B.M.} = \sqrt{1(1+2)} \text{ B.M.} = \sqrt{3} \text{ B.M.} = 1.73 \text{ B.M.}$

Ex.c. In F_2 (18e-s), the total number of electrons will be 18, PD = 18, hence, unpaired electron $n = I (18 - \text{total e-s}) I = I (18-18) I = 0$, magnetic moment, $\mu_s = \sqrt{n(n+2)} \text{ B.M.} = \sqrt{0(0+2)} \text{ B.M.} = 0 \text{ B.M.} = \text{Diamagnetic in nature.}$

F-3(For Set-3) - for the determination of number of unpaired electrons (n) of molecules or ions having total number of electrons 20: In this case, the number of unpaired electrons $n = [I (20 - \text{total e-s}) I]$

Ex.d. In Ne_2 (20e-s), the total number of electrons will be 20, hence, unpaired electron $n = I (20 - \text{total e-s}) I = I (20-20) I = 0$, and magnetic moment, $\mu_s = \sqrt{n(n+2)} \text{ B.M.} = \sqrt{0(0+2)} \text{ B.M.} = 0 \text{ B.M.} = \text{Diamagnetic in nature.}$

Adequate examples on the prediction of bond order of homo and heteronuclear diatomic molecules or ions having the total number of electrons fall in the range (1-20) without molecular orbital theory discussed in chapter 4 have been explored here also in Table 4.4.

Table 4.4 Bond order of diatomic species having (1-20) electrons

Species (Molecules or ions)	Total Number of e ^s (n)	Bond-Order (B.O.)
Bond-Order Values for the species having (1-2) e^s; Bond order = n/2		
H ₂ ⁺	1	0.5
H ₂ , He ₂ ²⁺	2	1
Bond-Order Values for the species having (2-6) e^s; Bond order = I 4- n I / 2		
H ₂ ⁻ , He ₂ ⁺	3	0.5
He ₂ ,	4	0
Li ₂ ⁺ , He ₂ ⁻	5	0.5
Li ₂ , He ₂ ²⁻ , Be ₂ ²⁺	6	1
Bond-Order Values for the species having (6-14) e^s; Bond order = I 8- n I / 2		
Be ₂ ⁺ , Li ₂ ⁻	7	0.5
Be ₂ , Li ₂ ²⁻	8	0
Be ₂ ⁻ , B ₂ ⁺	9	0.5
B ₂ , Be ₂ ²⁻ , HF	10	1
B ₂ ⁻ , C ₂ ⁺	11	1.5
C ₂ , B ₂ ²⁻ , N ₂ ²⁺ , CN ⁺	12	2
C ₂ ⁻ , N ₂ ⁺	13	2.5
N ₂ , CO, NO ⁺ , C ₂ ²⁻ , CN ⁻ , O ₂ ²⁺	14	3
Bond-Order Values for the species having (14-20)e^s ; Bond order = (20-n) / 2		
N ₂ ⁻ , NO, O ₂ ⁺	15	2.5
NO ⁻ , O ₂	16	2
O ₂ ⁻	17	1.5
F ₂ , O ₂ ²⁻ , HCl	18	1
F ₂ ⁻	19	0.5
Ne ₂	20	0

Table 5.5 Magnetic moments (μ_s) in B.M. of diatomic species

Species (Molecules or ions)	Total Number of e ^s	Number of unpaired electrons (n)	Magnetic moment (μ_s) in Bohr Magneton (B.M.)	Remark on magnetic behavior
H ₂ ⁺	1	1	1.73	Para magnetic
H ₂ , He ₂ ²⁺	2	0	0	Diamagnetic
H ₂ ⁻ , He ₂ ⁺	3	1	1.73	Para magnetic
He ₂ ,	4	0	0	Diamagnetic
Li ₂ ⁺ , He ₂ ⁻	5	1	1.73	Para magnetic

Q.6. Which of the following species is Paramagnetic? (CBSE AIPMT 1995)

- a) O_2^{2-} b) NO c) CO d) CN^-

Ans: b) NO

Q.7. Which of the following is not paramagnetic?

- a. NO b. F_2 c. O_2^- d. N_2^-

Ans: b. F_2 (All electrons in BMOs and ABMOs are paired)

Q.8. Paramagnetism is exhibited by molecules which

- a. Are not attracted by magnetic field b. Contain only paired electrons c. Contain unpaired electrons
d. Carry positive charge.

Ans: b. Contain only paired electrons

Q.9. Which of the following species is paramagnetic?

- a. CO_2 b. NO c. O_2^{2-} d. CN^-

Ans: b. NO (contains unpaired electron in ABMO $\pi^*_{2px}{}^1$)

Q.10. O_2 molecule is

- a. Paramagnetic b. Diamagnetic c. Ferromagnetic d. None of these

Ans: a. Paramagnetic

Q.11. The molecule having one unpaired electron is

- a. NO b. CO_2 c. CN^- d. O_2

Ans: a. NO, one unpaired electron in ABMO, π^*_{2px} (E.C. of NO is $\sigma_{1s}^2, \sigma_{1s}^{*2}, \sigma_{2s}^2, \sigma_{2s}^{*2}, \sigma_{2pz}^2, \pi_{2px}^2, \pi_{2py}^2, \pi^*_{2px}{}^1$)

Q.12. Which of the following species is paramagnetic?

- a. O_2^- b. CN^- c. CO d. NO^+

Ans: a. O_2^- (E.C. of O_2^- is $\sigma_{1s}^2, \sigma_{1s}^{*2}, \sigma_{2s}^2, \sigma_{2s}^{*2}, \sigma_{2pz}^2, \pi_{2px}^2, \pi_{2py}^2, \pi^*_{2px}{}^2, \pi^*_{2py}{}^1$)

Q.13. Which of the following molecular species has unpaired electron(s)?

- a. N_2 b. F_2 c. O_2^- d. O_2^{2-}

Ans: c. O_2^- (E.C. of O_2^- is $\sigma_{1s}^2, \sigma_{1s}^{*2}, \sigma_{2s}^2, \sigma_{2s}^{*2}, \sigma_{2pz}^2, \pi_{2px}^2, \pi_{2py}^2, \pi^*_{2px}{}^2, \pi^*_{2py}{}^1$)

Q.14. According to molecular orbital theory, which of the following statements about the magnetic character and bond order is correct regarding O_2^+ .

- a. Paramagnetic and bond order $< O_2$ b. Paramagnetic and bond order $> O_2$
c. Diamagnetic and bond order $< O_2$ d. Diamagnetic and bond order $> O_2$

Ans: b. Paramagnetic and bond order $> O_2$

Q.15. The molecule which contains an odd electron is (STGT 2017)

(a) O_2 (b) NO (c) CO (d) H_2S

Ans: (b) NO [In NO, total electrons = 15, hence it belongs to set 1: $(13-16)e^-$ s, where, $ND = 14$, hence number of unpaired electrons, $n = |ND - \text{total } e^-s| = |14 - 15| = 1$] (see **Table 5.5**)

Conclusion

It may be expected that these time economic innovative mnemonics, related to the prediction of magnetic properties without molecular orbital theory described in this chapter will be helpful for students and educators in inorganic chemical education at Undergraduate, Senior Undergraduate and Post-Graduate level to predict the magnetic moment of homo and heteronuclear molecules or ions without drawing electronic configuration of diatomic species. **Experiments, *in vitro*, on 100 students, showed that, by using these innovative formulae, students can save up to 10-15 minutes' time in the examination hall to solve different problems related to magnetic properties.** Based on this, I can strongly recommend using these time economic innovative mnemonics in inorganic chemistry.

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