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Bond-order and Magnetic Behavior of Diatomic Species without Molecular Orbital Theory

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Abstract In this chapter text based learning approaches has been highlighted by innovative and time economic way to enhance interest of students' who belong to paranoia zone in Electronic Structure of Atoms and Molecules beneath Inorganic Chemistry of chemical science. In this pedagogical survey, I have tried to hub two (02) time economic pedagogies by including seven (07) new formulae in the field of chemical education. This chapter explores the results and gives implications for context based teaching, learning and assessment.

Keywords: *general public, high school, graduate student, chemical bonding, bond order, paramagnetic, diamagnetic, molecular orbital theory*

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1. Introduction

The conventional methods [1-5] for prediction of bond order and magnetic properties of diatomic species having (1-20)e$^-$s using molecular orbital theory is time consuming. Keeping this in mind, I have introduced some innovative methods [6-12] in this book chapter to make chemistry metabolic, time economic and interesting.

2. Bond-Order of Diatomic Species without MOT

Bond-order usually predicted from the Molecular Orbital Theory. Molecular Orbital Theory (M.O.T.) was first proposed by Friedrich Hund and Robert Mulliken in 1933. They developed an approach to covalent bond formation which is based upon the effects of the various electron fields upon each other and which employs molecular orbital rather than atomic orbital. Each such orbital characterizing the molecule as a whole is described by a definite combination of quantum numbers and possesses relative energy value.

For homo and hetero nuclear diatomic molecules or ions having (1-20)e$^-$s.

The graphical representation presented in Figure 1 shows that bond-order gradually increases to 1 in the range (0-2) electrons then falls to zero in the range (2-4) electrons then it further rises to 1 for (4-6) electrons and once again falls to zero for (6-8) electrons then again rises to 3 in the range (8-14) electrons and then finally falls to zero for (14-20) electrons. For total no of electrons 2, 6 and 14, we may use multiple formulae, because they fall in the overlapping region in which they intersect with each other.

Graphical Representation of B.O. with number of electrons:

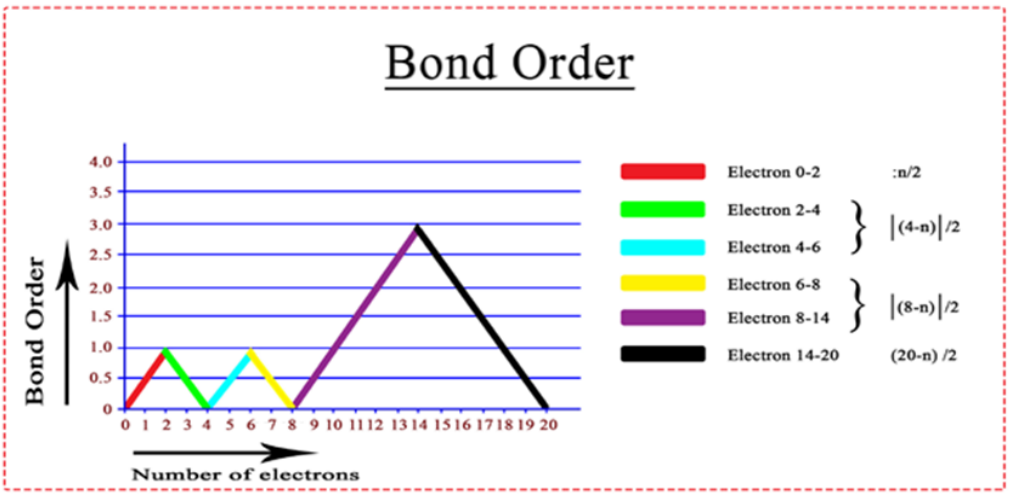

Figure 1. (B.O. vs number of electrons)

First of all we classify the molecules or ions into the following four (4) types based on total number of electrons present in them.

i) Molecules and ions having total no of electrons within the range (1-2):

In such case **Bond order = n/2;** [Where n = Total no of electrons]

Eg. H_2 (Total e⁻s = 2), Therefore B.O. = n/2 = 2/2 = 1.

ii) Molecules and ions having total no of electrons within the range (2-6):

In such case Bond order = I 4- n I / 2 ;

[Where n = Total no of electrons, 'I I' indicates Mod function i.e. the value of bond order is always positive]

Eg. Li_2^+(5e⁻s) Therefore B.O. = I 4-5 I / 2 = 1/2 = 0.5.

iii) Molecules and ions having total no of electrons within the range (6-14):

In such case Bond order = I 8-n I / 2

Eg: CO (Total e⁻s = 6+8=14), Therefore B.O.= I 8-14I/2 = 3.

iv) Molecules and ions having total no of electrons within the range (14-20):

In such case Bond order = (20-n) / 2 ; [Where n = Total no of electrons]

Eg. NO (Total e⁻s = 15), Therefore B.O. = 20-15/2 = 2.5.

Bond order prediction with examples have been represented in Table 1.

Relation of Bond order with Bond length, Bond Strength, Bond energy, Thermal stability and Reactivity

B.O. α 1 / Bond length or Bond distance;
B.O. α Bond strength;
B.O. α Bond Energy;
B.O. α Thermal Stability;
B.O. α 1 / Reactivity

By using the above relations one can easily predict, order of bond length/bond strength/bond energy/thermal stability/reactivity by conniving the bond order value for the above cited diatomic species in a time economic way.

Magnetic Behavior of Diatomic Species Without MOT

The present study involves three new formulae by just manipulating the number of unpaired electrons (n) using mod function (based on Applied Mathematics) and by means of these n values one can easily stumble the magnetic moment values in Bohr-Magneton 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 of all we 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 20 e⁻s

Table 1. ond order of diatomic species having

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

Then for different set we have to use three different formulae to calculate the number of unpaired electrons which have been presented in Table 2 and thus magnetic moment (μ_s in B.M.) can be evaluated in the following way:

F-1(For Set-1) - for the determination of number of unpaired electrons (n) of molecules or ions having 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 - total e⁻s) I]

Here, ND = next digit i.e. digit next to minimum digit and 'I I' indicates mod function.

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

Eg. He_2^+ (3e⁻s), the total number of electrons will be 3, ND = 2, Hence, unpaired electron n = I (ND - total e⁻s) I = I (2-3) I = 1. Hence, Magnetic Moment $\mu_s = \sqrt{n(n+2)}$ B.M. = $\sqrt{1(1+2)}$ BM = $\sqrt{3}$ BM = 1.73BM.

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-total e⁻s) I]; [I (6- total e⁻s)I] [I (8- total e⁻s) I] and [I (14- 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 - total e⁻s) I]

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

Eg: for C_2^- (13e⁻s), the total number of electrons will be 13, PD = 12

Hence, unpaired electron n = I (12 - total e⁻s) I = I (12-13) I = 1

Hence, Magnetic Moment $\mu_s = \sqrt{n(n+2)}$ B.M. = $\sqrt{1(1+2)}$ BM = $\sqrt{3}$ BM = 1.73BM

For F_2 (18e⁻s), the total number of electrons will be 18, PD = 18

Hence, unpaired electron n = I (18 - total e⁻s) I = I (18-18) I = 0

Hence, Magnetic Moment $\mu_s = \sqrt{n(n+2)}$ B.M. = $\sqrt{0(0+2)}$ BM = 0 BM = 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 - total e⁻s) I]

Eg: for Ne_2 (20e⁻s), the total number of electrons will be 20,

Hence, unpaired electron n = I (20 - total e⁻s) I = I (20-20) I = 0

Hence, Magnetic Moment $\mu_s = \sqrt{n(n+2)}$ B.M. = $\sqrt{0(0+2)}$ BM = 0 BM = Diamagnetic in nature.

Table 2. Magnetic Behaviour 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
Li_2, He_2^{2-}, Be_2^{2+}	6	0	0	Diamagnetic
Be_2^+,Li_2^-	7	1	1.73	Para magnetic
Be_2,Li_2^{2-}	8	0	0	Diamagnetic
Be_2^-,B_2^+	9	1	1.73	Para magnetic
B_2, Be_2^{2-}, HF	10	2	2.82	Para magnetic
B_2^-,C_2^+	11	1	1.73	Para magnetic
C_2,B_2^{2-},N_2^{2+}, CN^+	12	0	0	Diamagnetic
C_2^-,N_2^+	13	1	1.73	Para magnetic
N_2,CO,NO^+,C_2^{2-},CN^-,O_2^{2+}	14	0	0	Diamagnetic
N_2^-,NO,O_2^+	15	1	1.73	Para magnetic
NO^-,O_2	16	2	2.82	Para magnetic
O_2^-	17	1	1.73	Para magnetic
F_2,O_2^{2-},HCl	18	0	0	Diamagnetic
F_2^-	19	1	1.73	Para magnetic
Ne_2	20	0	0	Diamagnetic

3. Conclusions

It may be expected that these innovative methods would go a long way to help to the students of chemistry at Undergraduate, Senior Undergraduate and Post-Graduate level who would choose the subject as their career. Experiment *in vitro* on 100 students showed that by using these new innovative methods students can save up to 30-40 mins time in the examination hall. On the basis of this, I can strongly recommend to use these new time economic interesting pedagogies.

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