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NEW METHODS FOR THE PREDICTION OF MAGNETIC MOMENT OF HOMO AND HETERO NUCLEAR MONO AND DIATOMIC MOLECULES OR IONS WITHOUT MOT-A RAPID INNOVATIVE APPROACH

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Abstract: Prediction of magnetic moment without M.O.T. is of vital important tool to students of applied chemistry for solving different kinds of problems related to magnetic behavior. In this manuscript I try to present a simplest time saving innovative method for the identification of magnetic behavior of homo and hetero nuclear mono and diatomic molecules or ions having total electrons (01-20) excluding MOT concept. This method is not applicable for polyatomic molecules such as BCl3, CCl4, SO2 etc.

KeyWords

MOT-A,MAGNETIC BEHAVIOUR,Molecules,bond-order

Introduction:

The conventional method of determination of bond order and magnetic behavior using M.O.T.[1,2,3,4,5] is time consuming. Keeping this in mind, earlier a new innovative method[6] was introduced for the determination of magnetic behaviour of mono and diatomic molecules or ions having total electrons (01-20). The present method is the periodical part of the earlier method[6], so that student can forecast magnetic moment thus magnetic behavior of mono and diatomic molecules or ions having total electrons (01-20) without M.O.T..

Earlier eight (08) new innovative methods including seventeen (17) new formulae have been introduced on the easy prediction of 'Bond-Order of mono and diatomic homo and heteronuclear molecules or ions', 'Bond-order of oxide based acid radicals', 'Hybridization', 'IUPAC nomenclature of spiro and bicyclo compounds, 'spin multiplicity value calculation and prediction of magnetic properties of diatomic hetero nuclear molecules and ions, 'Aromaticity', 'magnetic properties of homo and hetero nuclear diatomic molecules and ions and 'simultaneous equations as a tool in the spectrophotometric analysis of two non-interacting substances in a binary mixture'[6-13]. The present study involves four new formulae by just manipulating the number of unpaired electrons (n) using mod function 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.

I think it would go a long way to help the students of In-organic chemistry who would choose the subject as their carrier. Experiment *in vitro* on 100 number of students show that by using these new innovative methods strike rate is 1Q/5secs.

On the basis of this, I can strongly recommend that this one be the most rapid method for the prediction of magnetic moment of homo and hetero nuclear mono and diatomic molecules or ions having total electrons (01-20) without MOT.

Result and discussions:

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

Then for different set we have to use four 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:

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)e⁻s, (3-5)e⁻s, (5-7)e⁻s, (7-10)e⁻s 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.

Therefore, for 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 and 8 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. These are shown in table-1.

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-5) - 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:-1

(Magnetic moments of homo and hetero nuclear mono and diatomic molecules or ions)

Molecules or ions	Total Number of e⁻s	n value (no of unpaired electrons)	Magnetic moment (μ_s) in BM	Remarks
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

Conclusions

In conclusion here I approach a new rapid innovative method on easier calculation of number of unpaired electrons and thus magnetic moment in BM. This new method is very helpful to undergraduate and graduate level students of chemistry. By using these methods student can easily predict nature of magnetic behaviour without MOT in a very simple and metabolic way.

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