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A Rapid and Innovative Method for the Easy Prediction of Magnetic Behavior of Homo and Hetero Nuclear Mono and Diatomic Molecules Or Ions without Mot

KEYWORDS: Total electrons, bond order, fractional number, positive integer, number of unpaired electrons

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ABSTRACT *Prediction of magnetic state is of vital important tool to students of applied chemistry for solving different kinds of problems related to magnetic behavior and also magnetic moment. In this manuscript I try to present an 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 in a very simple and time savings manner.*

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[10] was introduced for the determination of bond order of mono and diatomic molecules or ions having total electrons (01-20) from which we can easily predict the magnetic behavior of different kinds of homo and hetero nuclear mono and diatomic molecules or ions. The present method is the periodical part of the earlier method[10], so that student can forecast bond-order including magnetic behavior of mono and diatomic molecules or ions having total electrons (01-20) without M.O.T..

Previously eight innovative methods including twelve new formulae have been introduced on 'Hybridization', 'IUPAC nomenclature of spiro and bicyclo compounds', 'Bond Order of oxide based acid radicals', 'Bond order of mono and diatomic molecules or ions having total number of (1-20)e-s' and 'spin multiplicity value calculation and prediction of magnetic properties of diatomic hetero nuclear molecules and ions[6,7,8,9,10] for the benefit of students.

New important findings in case of Magnetic behavior of homo and hetero nuclear mono and diatomic molecules or ions:

Before introducing into innovative method for the prediction of magnetic behavior, first of all we shepherd the species (molecules and ions) with respect to their total number of electrons and bond order (Table-1).

Table -1
(Magnetic properties of homo and hetero nuclear mono and diatomic molecules or ions)

Molecules or ions	Total Number of e-s	B.O.	Magnetism	Remarks on Bond-Order
H_2^+	1	0.5	Para magnetic	Fractional
H_2, He_2^{2+}	2	1	Diamagnetic	+ve integer
H_2^-,He_2^+	3	0.5	Para magnetic	Fractional
He_2,	4	0	Diamagnetic	+ve integer
Li_2^+,He_2^-	5	0.5	Para magnetic	Fractional
Li_2, He_2^{2-}, Be_2^{2+}	6	1	Diamagnetic	+ve integer
Be_2^+,Li_2^-	7	0.5	Para magnetic	Fractional
Be_2,Li_2^{2-}	8	0	Diamagnetic	+ve integer
Be_2^-,B_2^+	9	0.5	Para magnetic	Fractional
B_2, Be_2^{2-}, HF	10	1	Para magnetic	Exception
B_2^-,C_2^+	11	1.5	Para magnetic	Fractional
C_2,B_2^{2-},N_2^{2+}, CN^+	12	2	Diamagnetic	+ve integer
C_2^-,N_2^+	13	2.5	Para magnetic	Fractional
N_2,CO,NO^+,C_2^{2-} ,CN^-,O_2^{2+}	14	3	Diamagnetic	+ve integer
N_2^-,NO,O_2^+	15	2.5	Para magnetic	Fractional
NO^-,O_2	16	2	Para magnetic	Exception
O_2^-	17	1.5	Para magnetic	Fractional
F_2,O_2^{2-},HCl	18	1	Diamagnetic	+ve integer
F_2^-	19	0.5	Para magnetic	Fractional
Ne_2	20	0	Diamagnetic	+ve integer

In most of the cases generally it is observed that the species having fractional bond-order will be paramagnetic in nature and the species having positive integer bond-order (i.e. bond order = 0,1,2,3 etc) will be diamagnetic in nature. But there is some exception focused in two cases during prediction of magnetic behavior of species having total number of electrons 10 and 16 respectively. In both the cases although they have positive integer bond-order values, 1 and 2, but they are paramagnetic in nature instead of diamagnetic.

Explanation on Exception behavior:

Species having total number of electrons 10 and 16 will be paramagnetic in nature although they have a positive integer bond order value. In this case, first, we have to predict their magnetic behavior from their magnetic moment values by calculating the number of unpaired electrons by the following two formulae based on bond-order.

New two formulae for resolving the number of unpaired electrons (n) based on bond-order in case of paramagnetic substances having total number of electrons 10 and 16.

When total number of electrons is 10
[The number of unpaired electrons (n) = 2 x bond order]

Eg: B_2, HF:- [10 electrons, B.O. = 1.0; n = 2 x bond order = 2 x 1.0 = 2.0,

Magnetic moment $\mu_s = \sqrt{n(n+2)}$ B.M. = $\sqrt{2(2+2)}$B.M. = $\sqrt{8}$ B.M. = 2.83B.M.]

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2. When total number of electrons is 16
[The number of unpaired electrons (n) = bond order]
Eg: O_2, NO^- etc. :- [16 electrons, B.O. = 2.0; n = bond order = 2, Magnetic Moment using spin only formula $\mu_s = \sqrt{n(n+2)}$ B.M. = $\sqrt{2(2+2)}$B.M. = $\sqrt{8}$ B.M. = 2.83B.M.]

CONCLUSIONS: It is expected that these innovative methods for the prediction of magnetic properties would go a long way to help to the students of chemistry and also applied chemistry that would choose the subject as their carrier. Experiment *in vitro* on 100 students show that for determination of B.O., using MOT, strike rate is 1Q/3min and by using these new innovative methods strike rate is 1Q/10secs. On the basis of this experiment I can strongly recommend to use these new methods for the prediction of magnetic behavior.

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REFERENCE R.L.Dutta, Inorganic Chem., 6th ed. (Part-1), p146-147, (2009) | 2. Lee.J.D., Concise Inorg. Chem, 5th ed.; Wiley India, (2009) | 3. Douglas.B., Mcdaniel. D. and Alexander.J., Concepts and Models of Inorg.Chem., 3rd | ed.; Wiley India, p157, (2007) | 4. Cotton.F.A.,Wilkinson.G.and Gaus.P.L.,Basic Inorg.Chem.,3rd ed.;Wiley India, p107,(2007) | 5. Mahan. B.M. and Meyers.R.J., International Student Edition University Chemistry,4th | ed.(1998) | 6. Das Arijit, 'Indian Journal of Applied Research', 03(07), p114, July 2013, ISSN-2249-555X | 7. Das Arijit, 'Indian Journal of Applied Research', 03(07), p594, July 2013, ISSN-2249-555X | 8. Das Arijit, 'Indian Journal of Applied Research', 03 (07), p596,July 2013, ISSN-2249-555X | 9. Das Arijit, 'Indian Journal of Applied Research', 03(08), p67,Aug 2013, ISSN-2249-555X | 10. Das Arijit,'Indian Journal of Applied Research',03(09), p63,Sept 2013, ISSN-2249-555X |