New Innovative Methods for Determination of Spin Multiplicity, Spin State and Magnetic Properties of Diatomic Hetero Nuclear Molecules or Ions in a Very Short Interval of Time

KEYWORDS unpaired electrons, upward arrow, downward arrow, alignment, diatomic, hetero nuclear molecules, even no of electrons, odd no of electrons

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ABSTRACT *Evaluation of spin-multiplicity value is a vitally important tool for prediction of spin state of atoms, molecules, ions or co-ordination complexes to students of chemistry in undergraduate, graduate and also in post-graduate level students for solving different kinds of problems. This new innovative method has to be introduced for the calculation of spin-multiplicity value in the easiest way by ignoring the calculation of total spin quantum number (S = Σs). Another method has also to be introduced for resolving magnetic nature of diatomic heteronuclei molecules or ions in a very simple way.*

INTRODUCTION

The method which is generally used[1,2,3,4,5] for the prediction of spin multiplicity value [(2S+1), where S = Σs = total spin quantum no] is time consuming. To keep the matter in mind a new innovative method has to be introduced for calculation of spin-multiplicity value in the easiest way by ignoring the calculation of total spin quantum number (S = Σs). Another method has also to be introduced for resolving magnetic behavior of diatomic hetero nuclear molecules or ions like CO, NO, NO^+, NO^-, CN, CN^- etc. in a very simple way. Another three innovative methods earlier introduced on the easy prediction of 'Hybridization', 'Bond-Order' and 'IUPAC nomenclature of spiro and bicyclo compounds[6,7,8] for the benefit of students.

These new innovative methods would go a long way to help to the students of chemistry who would choose the subject as their career. Experiment in vitro on 100 number of students show that for determination of spin multiplicity value using old (2S + 1) rule, strike rate is 1Q/3min and by using these new innovative methods strike rate is 1Q/5secs. On the basis of this experiment I can strongly recommend that these new methods will be the very rapid one for the determination of spin-multiplicity value and its corresponding spin-state (Table-1) by ignoring the calculation of total spin quantum number (S = Σs) in (2S + 1) rule.

New innovative methods for determination of spin multiplicity:

First of all we should classify the species (atoms, molecules, ions or complexes) for which spin multiplicity should be evaluated into three types based on the nature of alignment of unpaired electrons present in them.

a) Species having unpaired electrons alignment upward arrow (↑):

In this case, spin multiplicity = (n+1); where n = number of unpaired electrons.

↑		

Spin multiplicity = (n +1) = (1+1) = 2 (spin state = doublet)

↑	↑	

Spin multiplicity = (n +1) = (2+1) = 3 (spin state = triplet)

↑	↑	↑

Spin multiplicity = (n +1) = (3 + 1) = 4 (spin state = quartet)

↑↓	↑	↑

Spin multiplicity = (n +1) = (2 + 1) = 3 (in this case ignore paired electrons) (spin state = triplet)

↑↓	↑↓	↑

Spin multiplicity = (n +1) = (1 + 1) = 2 (spin state = doublet)

↑↓	↑↓	↑↓

Spin multiplicity = (n +1) = (0 + 1) = 1 (spin state = singlet)

b) Species having unpaired electrons alignment downward arrow (↓):

In this case spin multiplicity = (-n+1); where n = number of unpaired electrons. Here (-ve) sign indicate downward arrow.

↓		

Spin multiplicity = (-n +1) = (-1 + 1) = 0
(where n = no of unpaired e^-s)

↓	↓	

Spin multiplicity = (-n +1) = (-2 + 1) = -1

↓	↓	↓

Spin multiplicity = (-n +1) = (-3 + 1) = -2

↑↓	↓	↓

Spin multiplicity = (-n + 1) = (-2 + 1) = -1(in this case ignore paired electrons)

↑↓	↑↓	↓

Spin multiplicity = (-n + 1) = (-1 + 1) = 0

c) Species having unpaired electrons alignment both upward and downward arrow

In this case spin multiplicity = [(+n) + (-n) + 1]; where n = number of unpaired electrons in each mode. Here, (+ve) sign indicate upward mode of arrow and (–ve) sign indicate downward mode of arrow.

↑	↓	

Here total no of unpaired electrons = 2 in which one having upward direction (+1) and other having downward mode (-1).

Hence Spin multiplicity = [(+n) + (-n) +1] = [(+1) + (-1) + 1] = 1 (spin state = singlet)

↑	↑	↓

Here the total no of unpaired electrons = 3 in which two unpaired electrons lie in upward (+2) and one unpaired electrons lie in downward (-1) .

Hence Spin multiplicity = [(+n) + (-n) + 1] = [(+2) + (-1) + 1] = 2 (spin state = doublet)

↑	↓	↑	↓	↑

Here the total no of unpaired electrons = 5 in which three unpaired electrons lie upward (+3) and two unpaired electrons lie downward (-2) .

Hence Spin multiplicity = [(+n) + (-n) + 1] = [(+3) + (-2) +1] = 2 (spin state = doublet)

Table-1: spin multiplicity value and its corresponding spin state

Spin multiplicity value	Spin state
1	Singlet
2	Doublet
3	Triplet
4	Quartet
5	Quintet

New innovative method for determination of magnetic properties of diatomic heteronuclei molecules or ions:

In this case, first of all we have to count the total number of electrons with in the given species, then we isolate the species into two groups on the basis of even and odd no of total electrons present into them. It is generally observed that the species having even number of electrons (total electrons = even no) show diamagnetic character and the species having odd number of electrons (total electrons = odd no) show paramagnetic character (Table-2).

Table 2: Magnetic behavior of diatomic hetero nuclear molecules or ions

Molecules / ions	Total no of electrons (odd/even)	Magnetic behavior
CO	14 (even)	Diamagnetic
NO	15 (odd)	Paramagnetic
NO^+	14 (even)	Diamagnetic
NO^-	16 (even)	Diamagnetic
CN	13 (odd)	Paramagnetic
CN^-	14 (even)	Diamagnetic
CN^+	12 (even)	Diamagnetic
HCl	18 (even)	Diamagnetic
HF	10(even)	Diamagnetic

CONCLUSIONS: This article is very helpful to students in chemistry of undergraduate,

Graduate and also in Postgraduate level. These are the very time savings method. By using these methods student can predict spin state in a very simple way.

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REFERENCE 1. Lee.J.D., Concise Inorg. Chem, 5th ed.; Wiley Oxford, p944, p109-112, (2009). | 2. Douglas.B., Mcdaniel. D. and Alexander.J., Concepts and Models of Inorg.Chem., 3rd | ed.; Wiley India, p38, (2007). | 3. Cotton.F.A., Wilkinson.G.and Gaus.P.L.,Basic Inorg.Chem.,3rd ed.;Wiley India, | p523 & p111 (2007). | 4. Cotton. F.A., Chemical Applications of Group Theory, 3rd ed.; Wiley, New York 1990. | 5. Madan R.L.,Chem. for Degree students, 1st ed., p88(2011) ISBN-81-219-3533-4. | 6. Das Arijit, 'Indian Journal of Applied Research', 03(07), p114, July2013, ISSN-2249-555X | 7. Das Arijit, 'Indian Journal of Applied Research', 03(07), p594, July2013, ISSN-2249-555X | 8. Das Arijit, 'Indian Journal of Applied Research', 03 (07), p596, July2013, ISSN-2249-555X |