

# A Rapid and Innovative Method for Prediction of Spin Multiplicity and Spin State of Homo and Hetero Nuclear Diatomic Molecules and Ions within a Very Short Time

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**Abstract:** Determination of spin multiplicity is very important for identification of spin state of different molecules or ions. But, the conventional method of prediction of spin multiplicity by using formula  $(2S+1)$  is time consuming. So, in this manuscript, I tried to show a rapid and simple method for prediction of spin multiplicity value without calculating the total spin quantum number ( $S = \sum s$ ). This method is only applicable for homo and hetero nuclear diatomic molecules and ions having total electron (01-20).

**Keywords:** Even electron number, Molecules, Odd electron number, Spin Multiplicity value, Spin State, Total electron number, Value of 'l'.

## I. Introduction

The method of prediction of spin multiplicity is very important in inorganic chemistry. But the method which is generally used<sup>1-5</sup> for the prediction of spin multiplicity value  $[(2S+1)]$ , where  $S = \sum s$  = total spin quantum no] is time consuming. In various competitive examination, spin multiplicity related question plays a very important part. So, by using a rapid method, one can save their valuable time in exam hall. So, keeping all these things in mind, this new innovative method is introduced, which would go a long way to help all students. Another rapid method earlier introduced on easy prediction of 'Magnetic Moment'<sup>6</sup> for the benefit of students.

This method contains four(4) new formulae, with four(4) set of electron no. By placing only the value of 'l' (described as below)<sup>6</sup> in the respective formula, one can easily find the spin multiplicity value of different molecules and ions. So, we can use this rapid method in place of the conventional formula of finding spin multiplicity value represented as  $(2S+1)$ , where  $S = \sum s$  = total spin quantum no.

I believe, this rapid method will be very much helpful for all students, who are facing various competitive examination and by using these formulae, students can save their valuable time in exam hall.

So, on the basis of all these things, I can strongly recommend that this method will be most rapid method for the prediction of spin multiplicity value to identify spin state of homo and hetero nuclear diatomic molecules and ions having total electron no (01-20).

## II. Result And Discussions:

First of all, we take certain range of total electron of different molecules or ions, which are shown in four sets as follows.

Set-1:-Molecules or ions having (1-10 and 16)e<sup>-</sup>s ,(consider only even electron no. in this range)

Set-2:- Molecules or ions having (11-20, ≠16)e<sup>-</sup>s ,(consider only even electron no. in this range)

Set-3:- Molecules or ions having (1-8)e<sup>-</sup>s ,(consider only odd electron no. in this range)

Set-4:- Molecules or ions having (9-20)e<sup>-</sup>s ,(consider only odd electron no. in this range)

The above four sets, with their corresponding formulae are shown in table 1.

Table 1:-

Range of Total Electron No.	Formula
1-10 and 16 (consider only even 'e <sup>-</sup> ' no. in this range)	$2l+1$
11-20(≠16) (consider only even 'e <sup>-</sup> ' no. in this range without 16)	$2l-1$
1-8 (consider only odd 'e <sup>-</sup> ' no. in this range)	$l+2$
9-20 (consider only odd 'e <sup>-</sup> ' no. in this range)	$l+1$

### 2.1 Introduction to 'l' :

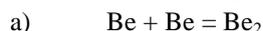
'l' is a variable, which can take only two value 0 or 1, depending on the total electron number of a molecule or ion.

If, the total electron no. for a molecule or ion lies between '1-8', then value of  $l = 0$ .

If, the total electron no. for a molecule or ion lies between '9-20', then value of  $l = 1$ .

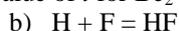
## 2.2 Source of conception behind the value of $l$ :

Actually this concept is taken from azimuthal quantum no.<sup>7,8</sup> in quantum chemistry, where we have found, for s orbital, quantum no  $l$  is taken as 0 ( $l$  is azimuthal quantum no.), for p orbital  $l$  is taken as 1. The same concept I have used here. If an atom contains only s orbital, the value of  $l$  is taken as 0, and if an atom contains s and p orbital both, then the value of  $l$  is taken as 1. The value of  $l$  depends on the two atom by which a diatomic molecule is composed. But in case of such diatomic molecule, where one atom has only s orbital and another atom has both s and p orbital, then I have observed if I take the atom consisting both s and p orbital in my consideration, then my experiment goes in a suitable way and give me a suitable result. But, if I take the atom, which has only s orbital, then my experiment does not give any suitable result. That's why, I have taken that atom in my consideration, which contains both s and p orbital in case of the ionic molecule or hetero nuclear diatomic molecule to find the value of  $l$ . After all, I have found, for the molecules which contains (1-8) total electron, the value of  $l$  for those molecules is 0, and for the molecules which contains (9-20) total electron, the value of  $l$  for those molecules is 1. E.g.:



Electronic configuration of Be :  $1S^22S^2$

We can observe that  $\text{Be}_2$  contain two Be (beryllium atom), and both Be atom contain only s orbital. So, the value of  $l$  for  $\text{Be}_2$  molecule is taken as 0.



Electronic configuration of H :  $1S^1$

Electronic configuration of F :  $1S^22S^22P^5$

We can observe that HF contains one H (hydrogen) atom and one F (fluorine) atom. And, H atom has only s orbital, whereas F atom has both s and p orbital. So, according to the considering rule, value of  $l$  is taken as 1.

### Discussion for set 1:

Total electron range : 1- 10 and 16 (consider only even electron no.)

In this case, Formula for spin multiplicity value =  $2l + 1$

Eg:  $\text{O}_2$ , which has total electron no. 16, therefore value of  $l = 1$ .

Hence, spin multiplicity value =  $2 \cdot 1 + 1 = 3$  (Triplet)

### Discussion for set 2:

Total electron range : 11- 20,  $\neq 16$  (consider only even electron no.)

In this case, Formula for spin multiplicity value =  $2l - 1$

Eg:  $\text{N}_2$ , which has total electron no. 14, therefore value of  $l = 1$ .

Hence, spin multiplicity value =  $2 \cdot 1 - 1 = 1$  (Singlet)

### Discussion for set 3:

Total electron range : 1- 8 (consider only odd electron no.)

In this case, Formula for spin multiplicity value =  $l + 2$

Eg:  $\text{Be}_2^+$ , which has total electron no. 7, therefore value of  $l = 0$ .

Hence, spin multiplicity value =  $0 + 2 = 2$  (Doublet)

### Discussion for set 4:

Total electron range : 9- 20 (consider only odd electron no.)

In this case, Formula for spin multiplicity value =  $l + 1$

Eg: NO, which has total electron no. 15, therefore value of  $l = 1$ .

Hence, spin multiplicity value =  $1 + 1 = 2$  (Doublet)

## III. Spin State

If, we can easily predict the spin multiplicity, then, we can easily isotate the spin state of different molecules and ions.

If spin multiplicity is 1, then spin state is 'Singlet'.

If spin multiplicity is 2, then spin state is 'Doublet'.

If spin multiplicity is 3, then spin state is 'Triplet'.

If spin multiplicity is 4, then spin state is 'Quartet'.

If spin multiplicity is greater than 4 ( $>4$ ), then spin state is 'Multiplet'

The spin multiplicity value of different molecules and ions with their spin state are shown in *table 2*.

Table 2

Different Molecules	Total Electron No.	Unpaired Electron No.	Value of 'l'	Spin multiplicity value using conventional formula (2S + 1)	Spin multiplicity value using new formula	Spin state
H <sub>2</sub>	2	0	0	2.0 + 1=1	2.0 + 1=1	Singlet
He <sub>2</sub>	4	0	0	2.0 + 1=1	2.0 + 1=1	Singlet
Li <sub>2</sub>	6	0	0	2.0 + 1=1	2.0 + 1=1	Singlet
Be <sub>2</sub>	8	0	0	2.0 + 1=1	2.0 + 1=1	Singlet
B <sub>2</sub>	10	2	1	$2(\frac{1}{2} + \frac{1}{2}) + 1=3$	2.1 + 1=3	Triplet
C <sub>2</sub>	12	0	1	2.0 + 1=1	2.1 - 1=1	Singlet
N <sub>2</sub>	14	0	1	2.0 + 1=1	2.1 - 1=1	Singlet
O <sub>2</sub>	16	2	1	$2(\frac{1}{2} + \frac{1}{2}) + 1=3$	2.1 + 1=3	Triplet
F <sub>2</sub>	18	0	1	2.0 + 1=1	2.1 - 1=1	Singlet
Ne <sub>2</sub>	20	0	1	2.0 + 1=1	2.1 - 1=1	Singlet
H <sub>2</sub> <sup>+</sup>	1	1	0	$2(\frac{1}{2}) + 1=2$	0 + 2=2	Doublet
H <sub>2</sub> <sup>-</sup>	3	1	0	$2(\frac{1}{2}) + 1=2$	0 + 2=2	Doublet
He <sub>2</sub> <sup>+</sup>	3	1	0	$2(\frac{1}{2}) + 1=2$	0 + 2=2	Doublet
Li <sub>2</sub> <sup>+</sup>	5	1	0	$2(\frac{1}{2}) + 1=2$	0 + 2=2	Doublet
Be <sub>2</sub> <sup>+</sup>	7	1	0	$2(\frac{1}{2}) + 1=2$	0 + 2=2	Doublet
HF	10	2	1	$2(\frac{1}{2}) + 1=2$	2.1 + 1=3	Triplet
C <sub>2</sub> <sup>+</sup>	11	1	1	$2(\frac{1}{2}) + 1=2$	1 + 1=2	Doublet
C <sub>2</sub> <sup>-</sup>	13	1	1	$2(\frac{1}{2}) + 1=2$	1 + 1=2	Doublet
N <sub>2</sub> <sup>+</sup>	13	1	1	$2(\frac{1}{2}) + 1=2$	1 + 1=2	Doublet
N <sub>2</sub> <sup>-</sup>	15	1	1	$2(\frac{1}{2}) + 1=2$	1 + 1=2	Doublet
O <sub>2</sub> <sup>+2</sup>	14	0	1	2.0 + 1=1	2.1 - 1=1	Singlet
O <sub>2</sub> <sup>-2</sup>	18	0	1	2.0 + 1=1	2.1 - 1=1	Singlet
O <sub>2</sub> <sup>-</sup>	17	1	1	$2(\frac{1}{2}) + 1=2$	1 + 1=2	Doublet
O <sub>2</sub> <sup>+</sup>	15	1	1	$2(\frac{1}{2}) + 1=2$	1 + 1=2	Doublet
NO <sup>+</sup>	14	0	1	2.0 + 1=1	2.1 - 1=1	Singlet
NO	16	2	1	$2(\frac{1}{2} + \frac{1}{2}) + 1=3$	2.1 + 1=3	Triplet
CN	13	1	1	$2(\frac{1}{2}) + 1=2$	1 + 1=2	Doublet
CN <sup>+</sup>	12	0	1	2.0 + 1=1	2.1 - 1=1	Singlet
CO <sup>+</sup>	15	1	1	$2(\frac{1}{2}) + 1=2$	1 + 1=2	Doublet

#### IV. Conclusion

After all, I approach a new innovative and rapid method for prediction of spin multiplicity value and their corresponding spin state. This method will be very much helpful for all students of chemistry. And by using this rapid method, one can easily predict the spin multiplicity value of different molecules and ions easily and also, students will be able to answer very rapidly in competitive examination of spin multiplicity related questions.

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