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New Innovative methods for prediction of Bond order of mono and diatomic molecules, ions and also acid radicals in a very short time

KEYWORDS Total electrons, Bond length, Bond strength, Bond dissociation energy, Thermal stability, Reactivity, Central atom/Peripheral atom, Charge on oxide based acid radical

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ABSTRACT : *Prediction of bond order is a vitally important to students of chemistry in undergraduate, graduate and also in Post-graduate level for solving different kinds of problems related bond length, bond strength, bond dissociation energy, thermal stability and reactivity. This new innovative method has to be introduced for calculation of bond order of mono and diatomic molecules and ions having total electrons (08-20) in a very simple way, which is also be a time savings one. Another method has also to be introduced for determination of bond order of oxide based acid radicals in a very simple way.*

INTRODUCTION

The method which is generally used based on M.O.T.[1,2,3,4,5] for determination of bond order is time consuming. To keep the matter in mind a new innovative method has to be introduced for calculation of bond order of molecules and ions having total electrons (08-20) in a very simple way, which is also be a time savings one. This method is not applicable for polyatomic molecules such as BF_3, CH_4, CO_2 etc.. and is applicable for mono atomic and diatomic molecules and ions such as CO, NO^+, O_2^{2+} etc . Another method has also to be introduced for determination of bond order of oxide based acid radicals in a very simple way.

These new innovative methods for prediction of hybridization states 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 B.O., using MOT, 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 bond order without M.O.T..

First of all one should <u>classify the molecules or ions into two types based on total no of electrons</u>.

a) Molecules and ions having total no of electrons with in the range (08-14).
Eg:Be_2(Total e^-s = 08),B_2(Total e^-s = 10), C_2(Total e^-s = 12),C_2^+ (Total e^-s = 12-1=11), C_2^-(Total e^-s = 12 +1=13), N_2(Total e^-s = 14), N_2^+ (Total e^-s = 13), O_2^{2+} (Total e^-s =16-02=14), CO (Total e^-s = 06+08=14), NO^+ (Total e^-s = 07+08-01=14).

b) Molecules and ions having total no of electrons with in the range (15-20).
Eg:N_2^- (Total e^-s = 14+01=15), O_2(Total e^-s = 16), O_2^+(Total e^-s = 15), O_2^- (Total e^-s = 17), O_2^{2-} (Total e^-s =16+02=18), F_2(Total e^-s = 18), Ne_2(Total e^-s = 20).

New Method for determination of Bond order of Melecules and Ions having total no of electrons with in the range (08-14)e^-s.

$$\text{In such case Bond order} = \frac{(N-8)}{2} \quad \text{[Where N = Total no of electrons]}$$

Eg:-

Be_2 (Total e^-s = 08), Therefore B.O. = 08-08/2 = 0 (Does not exist).

B_2 (Total e^-s = 10), Therefore B.O. = 10-08/2 = 1

C_2 (Total e^-s = 12), Therefore B.O. = 12-08/2 = 2

C_2^+ (Total e^-s = 12-1=11), Therefore B.O. = 11-08/2 = 1.5

C_2^- (Total e^-s = 12 +1=13), Therefore B.O. = 13-08/2 = 2.5

N_2 (Total e^-s = 14), Therefore B.O. = 14-08/2 = 3

N_2^+ (Total e^-s = 13), Therefore B.O. = 13-08/2 = 2.5

CO (Total e^-s = 06+08=14), Therefore B.O. =14-08/2 = 3

NO^+ (Total e^-s = 07+08-01=14), Therefore B.O. =14-08/2 = 3.

CN^+ (Total e^-s = 06+07-01=12), Therefore B.O. =12-08/2 = 2.

CN^- (Total e^-s = 06+07+1 =14), Therefore B.O. =14-08/2 = 3.

New Method for determination of Bond order of Melecules and Ions having total no of electrons with in the range (15-20)e^-s.

$$\text{In such case Bond order} = \frac{(20-N)}{2} \quad \text{[Where N = Total no of electrons]}$$

Eg:
N_2^- (Total e^-s = 14+01=15), Therefore B.O. = 20-15/2 = 2.5

O_2 (Total e^-s = 16), Therefore B.O. = 20-16/2 = 2

O_2^+ (Total e^-s = 15), Therefore B.O. = 20-15/2 = 2.5

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

O_2^- (Total e^-s = 17), Therefore B.O. = 20-17/2 = 1.5

O_2^{2-}(Total e^-s =16+02=18), Therefore B.O. = 20-18/2 = 1

F_2 (Total e^-s = 18), Therefore B.O. = 20-18/2 = 1

Ne_2 (Total e^-s = 20, Therefore B.O. = 20-20/2 = 0 (Does not exist).

New Method for determination of Bond order of oxide based Acid Radicals:
Incase of Acid Radicals
B.O.=Valency of Peripheral atom + (Charge on Acid Radical

/ Number of Peripheral

atoms)

Eg:

SO_4^{2-} ; (Valency of Peripheral atom i.e. Oxygen = 2, Charge on acid radical = -2, Number of Peripheral atoms = 04), Therefore B.O. = 2 + (-2/4) = (8 – 2)/4 = 6/4 = 3/2 = 1.5

SO_3^{2-} ; (Valency of Peripheral atom i.e.Oxygen = 2, Charge on acid radical = -2, Number of Peripheral atoms = 03), Therefore B.O. = 2 + (-2/3) = (6-2)/3 = 4/3 = 1.33

PO_4^{3-} ; (Valency of Peripheral atom i.e. Oxygen = 2, Charge on acid radical = -3, Number of Peripheral atoms = 04), Therefore B.O. = 2 + (-3/4) = (8 – 3)/4 = 5/4 = 1.25

NO_3^- ; (Valency of Peripheral atom i.e. Oxygen = 2, Charge on acid radical = -1, Number of Peripheral atoms = 03), Therefore B.O. = 2 + (-1/3) = (6 – 1)/3 = 5/3 = 1.66

NO_2^- ; (Valency of Peripheral atom i.e. Oxygen = 2, Charge on acid radical = -1, Number of Peripheral atoms = 02), Therefore B.O. = 2 + (-1/2) = (4 – 1)/2 = 3/2 = 1.5

BO_3^{3-} ; (Valency of Peripheral atom i.e. Oxygen = 2, Charge on acid radical = -3, Number of Peripheral atoms = 03), Therefore B.O. = 2 + (-3/3) = (6 – 3)/3 = 3/3 = 1

CO_3^{2-} ; (Valency of Peripheral atom i.e. Oxygen = 2, Charge on acid radical = -2, Number of Peripheral atoms = 03), Therefore B.O. = 2 + (-2/3) = (6 – 2)/3 = 4/3 = 1.33

ClO_4^- ; (Valency of Peripheral atom i.e. Oxygen = 2, Charge on acid radical = -1, Number of Peripheral atoms = 04), Therefore B.O. = 2 + (-1/4) = (8 – 1)/4 = 7/4 = 1.75

SiO_4^{4-}; (Valency of Peripheral atom i.e. Oxygen = 2, Charge on acid radical = - 4, Number of Peripheral atoms = 04), Therefore B.O. = 2 + (- 4/4) = 1

Relation of Bond order with Bond length, Bond Strength, Bond dissociation energy, Thermal stability and Reactivity.
B.O. α 1 / Bond length or Bond distance;

B.O. α Bond strength;
B.O. α Bond dissociation energy;
B.O. α Thermal Stability;
B.O. α 1 / Reactivity.

Problems based on Bond Order:

1. The pair of species with the same bond order is **(AIPMT-12)**
   a)O_2^{2-}, B_2 b)O_2^+, NO^+ c) NO, CO d)N_2, O_2

Ans: a) O_2^{2-}, B_2 both have bond order 1.

2. Bond order of 1.5 is shown by **(AIPMT-12)**
   a)O_2^+ b)O_2^- c)O_2^{2-} d)O_2.

Ans: b) O_2^-, bond order is 1.5

3. Using MOT predict which of the following species has the shortest bond length ?
   (AIEEE-09)
   a)O_2^{2+} b)O_2^+ c)O_2^- d)O_2^{2-}.

Ans: B.O. α 1 / Bond length; O_2^{2+} shows highest B.O. 3 i.e. shortest bond length.

4. Which one of the following pairs of species have the same bond order ? **(AIEEE-08)**
   a) CN^- and NO^+ b)CN^- and CN^+ c)O_2^- and CN^- d)NO^+ and CN^+.

Ans:- a) both are iso-electronic having 14 e^-s and same bond order 3.

5. Find out the bond order of O_2 and N_2 **(C.U. 06)**
   Ans: O_2, B.O. = 2, N_2, B.O. = 3.
6. Arrange the following in increasing order of bond length **(C.U. 92)**
   O_2, N_2, F_2

Ans: B.O. α 1 / Bond length; Hence Bond length order is N_2(BO=3) < O_2(BO=2) < F_2 (BO=1).

7. Find out the bond order of O_2^+, O_2 and O_2^- species. **(T.U. 09)**

Ans: B.O. of O_2^+ is 2.5, B.O. of O_2 is 2 and B.O. of O_2^- is 1.5.

8. Indicate the changes in bond order, bond distance to the following reactions: **(T.U.09)**
   i) $O_2 + 2e^- \rightarrow O_2^{2-}$
   ii) $N_2 - e^- \rightarrow N_2^+$
   iii) $NO \rightarrow NO^+ + e^-$

Ans: We know with increasing bond order bond length or Bond distance decreases.

i) $O_2 + 2e^- \rightarrow O_2^{2-}$;
changes of B.O. is 2 to 1 i.e. bond order decreases so bond distance increases.

ii) $N_2 - e^- \rightarrow N_2^+$;

changes of B.O. is 3 to 2.5 i.e. bond order decreases so bond distance increases.

iii) $NO \rightarrow NO^+ + e^-$;
changes of B.O. is 2.5 to 3 i.e. bond order increases so bond distance decreases.

CONCLUSIONS:
This article is very helpful to students in chemistry of undergraduate, graduate and also in Postgraduate level. This is one of the very time savings method. By using this method student can predict bond order in a very simple way.

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