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New Methods for Prediction of Bond Order of Mono and Diatomic Homo and Hetero Nuclear Molecules or Ions Having (1-20) E¯S and Oxide Based Acid Radicals Without Mot – A Rapid Innovative Approach

KEYWORDS: Total electrons, Central atom/Peripheral atom, Oxide based acid radical, Bond length, Bond strength, Bond dissociation energy, Thermal stability, Reactivity.

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ABSTRACT *Prediction of bond order is of vital important to students of chemistry for solving different kinds of problems related to bond length, bond strength, bond dissociation energy, thermal stability and reactivity. Keeping this in mind, a new innovative method is presented for calculation of bond order of molecules and ions having total electrons (01-20) in a very simple and time saving manner. This method is applicable for mono atomic and diatomic molecules and ions such as CO, NO+, O_2^{2+} etc. and is not applicable for polyatomic molecules such as BF_3, CH_4, CO_2 etc.*

Introduction
The conventional method of determination of bond order 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 bond order of mono and diatomic molecules or ions having total electrons (08-20). The present method with its graphical representation (Fig-1; b.o. vs total no of e^-s) is the periodical part of the earlier method[6] (08-20) e^-s, so that student can forecast bond-order of mono and diatomic molecules or ions having total electrons (01-20).This method is applicable for mono atomic and diatomic homo and hetero nuclear molecules and ions such as CO, NO^+, O_2^{2+} , H_2, H_2^+, H_2^-, He_2, He_2^+, He_2^-,Li_2, Li_2^+, Li_2^- etc. and not applicable for polyatomic molecules such as BF_3, CH_4, CO_2 etc.

The Graph

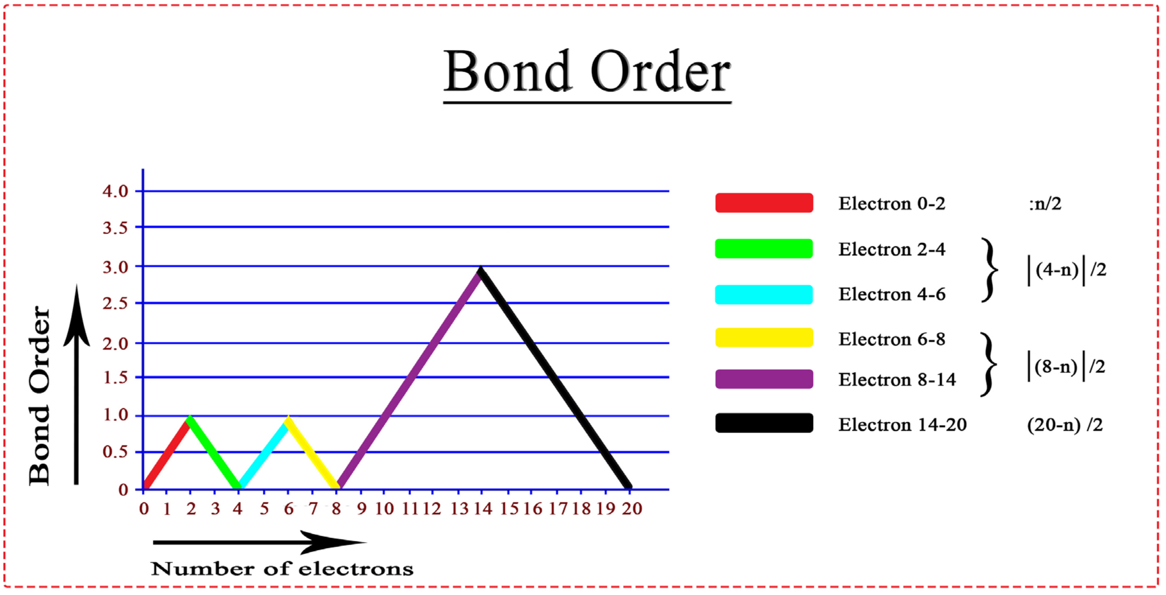

Fig-1: Bond-Order vs Total no of electrons.

The graphical representation presented in Fig. 1 shows that bond-order gradually increases to 01 in the range (0-02) electrons then it falls to zero in the range (02-04) electrons then it further rises to 01 for (04-06) electrons and once again falls to zero for (06-08) electrons then again rises to 3 in the range (08-14) electrons and then finally falls to zero for (14-20) electrons. For total no of electrons 2, 6 and 14, we use multiple formulae, because they fall in the overlapping region in which they intersect with each other. It is generally observed that in most of the cases for homo nuclear diatomic molecules or ions bond order will be fractional and it will also be paramagnetic in nature.

First of all we classify the molecules or ions into four (04) types based on the total no of electrons.

Molecules and ions having total no of electrons within the range (0-2).

In such case Bond order = n/2 ; [Where n = Total no of electrons]

Eg: H_2 (Total e^-s = 02), Therefore B.O. = n/2 = 02/2 = 1

H_2^+ (Total e^-s = 02-1 = 1), Therefore B.O. = n/2 = 01/2 = 0.5

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Molecules and ions having total no of electrons within the range (2-6).

In such case Bond order = I 4- n I / 2 ; [Where n = Total no of electrons, 'I I' indicates Mod function i.e. the value of bond order is always positive]

Eg. H_2 (2e^-s), H_2^- (3e^-s), He_2 (4e^-s) , He_2^+ (3e^-s), He_2^- (5e^-s),Li_2(6e^-s), Li_2^+(5e^-s)

H_2^- (3e^-s) Therefore B.O. = I 4-3 I / 2 = 1/2 = 0.5 (ionic species)

He_2 (4e^-s), Therefore B.O. = I 4-4 I / 2 = 0 (Does not exist)

Li_2^+(5e^-s) Therefore B.O. = I 4-5 I / 2 = 1/2 = 0.5 (ionic species)

Li_2(6e^-s) Therefore B.O. = I 4-6 I / 2 = 1

Molecules and ions having total no of electrons within the range (6-14).

In such case Bond order = I 8-n I / 2 ; [Where n = Total no of electrons, 'I I' indicates Mod function i.e. the value of bond order is always positive]

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).

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

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

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

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

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

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

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

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

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

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

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

Molecules and ions having total no of electrons within the range (14-20).

In such case Bond order = (20-n) / 2 ; [Where n = Total no of electrons]

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).

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

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 (ionic)

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 (ionic)

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).

Bond order of oxide based Acid Radicals
In case of Acid Radicals

B.O.=Valency of one of peripheral atom + (Charge on Acid Radical / Total number of peripheral atoms)

Eg:

SO_4^{2-} ; (Valency of one Peripheral atom i.e. Oxygen = 2, Charge on acid radical = -2, Total 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 one Peripheral atom i.e.Oxygen = 2, Charge on acid radical = -2, Total Number of Peripheral atoms = 03), Therefore B.O. = 2 + (-2/3) = (6-2)/3 = 4/3 = 1.33

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

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

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

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

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

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

ClO_3^- ; (Valency of one Peripheral atom i.e. Oxygen = 2, Charge on acid radical = -1, Total Number of Peripheral atoms = 03), Therefore B.O. = 2 + (-1/3) = (6 – 1)/3 = 5/3 = 1.66

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

Conclusions:
It is expected that these innovative methods for prediction of bond order 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 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 it can be strongly recommended to use these new metabolic methods.

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