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New Innovative Methods for Prediction of Bond Order of Mono and Diatomic Molecules or Ions Having Total Number of (1-20)E S In a Very Short Time

KEYWORDS: Total electrons, mod function, Bond length, Bond strength, Bond dissociation energy, Thermal stability, Reactivity

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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 relating to 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 (01-20) in a very simple way, which will really be a time saving one. Earlier another method has also to be introduced for the determination of bond order of mono and diatomic molecules or ions having total electrons (08-20). This new one (01-20) e-s will be the innovative part of the earlier one (08-20) e-s, so that students can predict bond-order of mono and diatomic molecules or ions having total electrons (01-20).*

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. Keeping the matter in mind earlier a new innovative method has been introduced[6] for the determination of bond order of mono and diatomic molecules or ions having total electrons (08-20). This new one, (01-20) e-s with its graphical representation (b.o. vs total no of e-s) will be the periodical part of the earlier method (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 not applicable for polyatomic molecules and is applicable for mono atomic and diatomic molecules and ions such as H_2, H_2^+, H_2^-, He_2, He_2^+, He_2^-,Li_2, Li_2^+, Li_2^- etc.

Other seven innovative methods including ten new formulae were earlier introduced on the easy prediction of 'Hybridization', 'IUPAC nomenclature of spiro and bicyclo compounds', 'spin multiplicity value calculation and prediction of magnetic properties of diatomic hetero nuclear molecules and ions' [7,8,9] for the benefit of students.

These new 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 I can strongly recommend that these new methods will be the very rapid one for the determination of bond order without M.O.T..

This new formulae, (01-20) e-s with its graphical representation (b.o.vs total no of e-s) will be the periodical part of the earlier method (08-20) e-s.

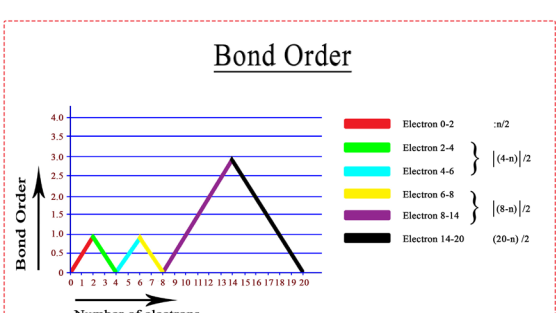

Fig: Bond-Order vs Total no of electrons.

From the above graphical representation we can easily explain the nature of the graph in the following way.

The graphical representation follow zig-zag nature. Bond-order gradually increases to 01 upto (0-02) electrons then it falls to zero upto (02-04) electrons then it further rises to 01 upto (04-06) electrons then fall to zero upto (06-08) electrons then again rises 3 upto (08-14) electrons then gradually fall to zero upto (14-20) electrons. For total no of electrons 2, 6 and 14, we use multiple formulae, becoz they fall in the overlapping region in which they intersect with each other and it is generally observed that for homonucler 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 total no of electrons.

a) 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

b) Molecules and ions having total no of electrons within the range (2-6).
In such case Bond order = |4- n| / 2 ; [Where n = Total no of electrons, | | 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. = |4-3| / 2 = 1/2 = 0.5 (ionic species)
He_2 (4e-s), Therefore B.O. = |4-4| / 2 = 0 (Does not exist)
Li_2^+(5e-s) Therefore B.O. = |4-5| / 2 = 1/2 = 0.5 (ionic species)
Li_2(6e-s) Therefore B.O. = |4-6| / 2 = 1

c) Molecules and ions having total no of electrons within the range (6-14).
In such case Bond order = |8-n| / 2 ; [Where n = Total no of electrons, | | indicates Mod function i.e. the value of bond order is always positive]
Eg. Be2(Total e-s = 08),B2(Total e-s = 10), C2(Total e-s = 12),C2+ (Total e-s = 12-1=11), C2-(Total e-s = 12 +1=13), N2(Total e-s = 14), N2+ (Total e-s = 13), O22+ (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. = |08-08| / 2 = 0 (Does not exist).

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

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

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

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

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

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

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

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

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

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

d) 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).

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.

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 saving methods. By using this method students can predict bond order in a very simple way.

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