# A Review of Time Economic Innovative Mnemonics in Chemical Education

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## Abstract

In this review article, formulae based mnemonics on chemical education have been highlighted by innovative and time economic way to enhance the interest of students' who belong to paranoia zone of chemistry. Here, I have tried to hub fifteen (15) time economic mnemonics by including thirty-six (36) formulae in the field of chemical education. This article encourages students to solve multiple choice type questions (MCQs) at different competitive examinations in time economic ground.

# Keywords

Hybridization, molecular orbital theory, bond order, magnetic properties, spin multiplicity, aromatic compounds, alkenes, and alkynes

•Received 6 July 2017 •Revised 26 October 2017 •Accepted 27 December 2017

# Introduction

The conventional methods for determination of hybridization of simple molecules including heterocyclic compounds, bond order of diatomic species having (1-20)e-s using M.O.T., bond-order of oxide-based acid radicals, prediction of spin state using spin multiplicity value, aromatic and anti-aromatic behavior of organic compounds, evaluation of magnetic behaviour of diatomic species having (1-20)e-s with M.O.T., calculation of number bonds in olefinic hydrocarbons and alkynes etc. is time-consuming (Pauling, 1931; Mulliken, 1972; Hall, 1991; Engel and Reid, 2006; Lee, 2009; Douglas, Mcdaniel and Alexander, 2007; Cotton, Wilkinson and Gaus, 2007; Mahan and Meyers, 1998; Finar, 2002, 2004; Morrison and Boyd, 1999; Solomons and Fryhle, 2012; Smith, 2008; Hückel, 1931; March, 1985; Badertscher, Bischofberger, Munk, Morton and Pretsch, 2001). Keeping this in mind, in this survey, I have introduced some innovative methods to make chemistry metabolic, time economic and interesting (Das, Paul, Sanjeev, and Jagannadham, 2014; Das, 2017; Das, Adhikari, Paul, Sanjeev, and Jagannadham, 2014; Das, Sanjeev and Jagannadham, 2014; Das, Sanjeev and Jagannadham, 2014). Here, I have tried to discuss them abruptly.

## **Time Economic Innovative Mnemonics**

## 1. Predicting The Hybridization of Simple Molecules

In chemistry, hybridization is the concept of mixing atomic orbitals into newly hybrid orbitals suitable for the pairing of electrons to form chemical bonds in valence bond theory (VBT). Hybrid orbitals are differing in energies, shapes, etc., than the component atomic orbitals. Hybrid orbitals are very useful in the explanation of molecular geometry and atomic bonding properties. Prof. Linus Pauling, first proposed the Hybridization in order to explain the structure of molecules such as methane (CH<sub>4</sub>) using atomic orbitals (Pauling, 1931).

## The conventional method for prediction of hybridization state:

Hybridization state for a molecule can be calculated by the formula 0.5 (V+H-C+A)

where, V = Number of valence electrons in central atom, H = Number of surrounding monovalent atoms, C = Cationic charge, A = Anionic charge

## Innovative time economic mnemonics for the prediction of hybridization state:

1.1. Prediction of sp, sp<sup>2</sup>, sp<sup>3</sup> Hybridization state:

Hybridization is nothing but the mixing of orbital's in different ratio and the newly mixed orbitals called hybrid orbitals. The mixing pattern is as follows:

s + p (1:1) - sp hybrid orbital; s + p (1:2) - sp<sup>2</sup> hybrid orbital; s + p (1:3) - sp<sup>3</sup> hybrid orbital

A formula used for the determination of sp, sp<sup>2</sup>, and sp<sup>3</sup> hybridization state:

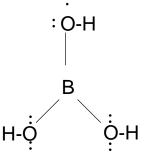
( 
$$^{Power \ on \ the \ Hybridization}_{state \ of \ the \ central \ atom}$$
 ) = (  $^{Total \ no \ of \ \sigma \ bonds}_{around \ each \ central \ atom}$  ) – 1

From the Lewis structure of a molecule, first of all, predict the number of sigma bonds ( $\sigma$ -bonds), pi bonds ( $\pi$ -bonds) or the lone electron pair of electrons (LPe-s) if any. All single (-) bonds are the  $\sigma$  bond, in the double bond (=) there is  $1\sigma$  and  $1\pi$ , in triple bond (=) there is  $1\sigma$  and  $2\pi$  (exclude  $\pi$  bond). In addition to these each lone pair (LP) and Co-ordinate bond ( $\rightarrow$ ) can be treated as  $1\sigma$  bond subsequently (Das, Sanjeev, and Jagannadham, 2014).

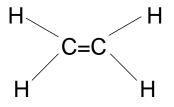
This translates into the following:

a. In NH<sub>3</sub>: central atom N is surrounded by three N-H single bonds i.e. three sigma ( $\sigma$ ) bonds and one lone pair (LP) i.e. one additional  $\sigma$  bond. So, in NH<sub>3</sub> there is a total of four  $\sigma$  bonds [3 bond pairs (BPs) + 1 lone pair (LP)] around central atom N. Therefore, in this case, power of the hybridization state of N = 4–1 = 3 i.e. hybridization state = sp<sup>3</sup>.

- b. In H<sub>2</sub>O: central atom O is surrounded by two O-H single bonds i.e. two sigma ( $\sigma$ ) bonds and two lone pairs i.e. two additional  $\sigma$  bonds. So, all together in H<sub>2</sub>O, there are four  $\sigma$ bonds (2 bond pairs + 2 lone pairs) around central atom O, So, in this case, power of the hybridization state of O = 4 – 1 = 3 i.e. hybridization state of O in H<sub>2</sub>O = sp<sup>3</sup>.
- c. In H<sub>3</sub>BO<sub>3</sub>:- B has 3 $\sigma$  bonds (3BPs but no LPs) and oxygen has 4 $\sigma$  bonds (2BPs & 2LPs) so, in this case, power of the hybridization state of B = 3-1 = 2 i.e. B is sp<sup>2</sup> hybridized in H<sub>3</sub>BO<sub>3</sub>. On the other hand, the power of the hybridization state of O = 4-1= 3 i.e. hybridization state of O in H<sub>3</sub>BO<sub>3</sub> is sp<sup>3</sup>.



- d. In I-Cl: I and Cl both have 4σ bonds and 3LPs, so, in this case, power of the hybridization state of both I and Cl=4–1=3 i.e. hybridization state of I and Cl both are sp<sup>3</sup>.
- e. In CH<sub>2</sub>=CH<sub>2</sub>: each carbon is attached with 2 C-H single bonds (2  $\sigma$  bonds) and one C=C bond (1 $\sigma$  bond). So, altogether there are 3 sigma bonds and in this case, the power of the hybridization state of both C=3–1 = 2 i.e. hybridization state of both C's are sp<sup>2</sup>.



# 1.2. Prediction of $sp^3d$ , $sp^3d^2$ , $sp^3d^3$ Hybridization state:

In case of sp<sup>3</sup>d, sp<sup>3</sup>d<sup>2</sup> and sp<sup>3</sup>d<sup>3</sup> hybridization state there is a common term sp<sup>3</sup> for which 4 sigma bonds are responsible. So, in addition to 4 sigma bonds, for each additional sigma, added one d orbital gradually as follows:-

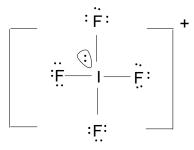
 $5\sigma$  bonds =  $4\sigma$  bonds + 1 additional  $\sigma$  bond = sp<sup>3</sup>d hybridization

 $6\sigma$  bonds =  $4\sigma$  bonds + 2 additional  $\sigma$  bonds =  $sp^3d^2$  hybridization

 $7\sigma$  bonds =  $4\sigma$  bonds + 3 additional  $\sigma$  bonds =  $sp^3d^3$  hybridization

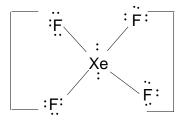
This translates into the following:

a. IF<sub>4</sub>+:

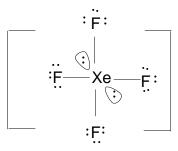


I have 7 e-s in its outermost shell, so, in this case, subtract one e- from 7 i.e. 7 - 1 = 6. So, out of 6 electrons, 4 electrons form 4 I-F bonds i.e. 4 sigma bonds and there is one LP. So, altogether there are 5  $\sigma$  bonds. So,  $5\sigma$  bonds = 4  $\sigma$  bonds + 1 additional  $\sigma$  bond = sp<sup>3</sup>d hybridization

b. XeF4:



Lewis Structure of XeF4:



Xe, an inert gas, consider 8 e-s in its outermost shell, 04 of which form 04 Xe-F sigma bonds and there are two LPs, i.e. altogether there is  $06 \sigma$  bonds =  $04 \sigma$  bonds + 02 additional  $\sigma$  bonds =  $sp^3d^2$  hybridization.

c. IF<sub>7</sub>: 7 I-F single bonds i.e.  $7\sigma$  bonds =  $4\sigma$  bonds + 3 additional  $\sigma$  bonds =  $sp^3d^3$  hybridization.

In case of determination of the hybridization state by using the above method, one must have a clear idea about the outermost electrons of different family members in the periodic table as follows:

Family	Outermost electrons
Carbon family	04
Nitrogen family	05
Oxygen family	06
Halogen family	07
Inert gas family	08

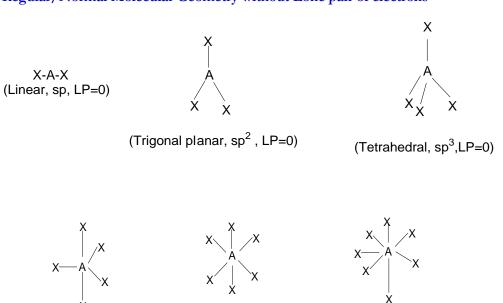
In case of cationic species, requisite electron/electrons must be removed from the outermost orbit of the central atom and in case of anionic species, added requisite electron with the outermost electrons of the central atom. Examples have been explored in Table 1.

#### Table 1. $\sigma$ bonds and corresponding hybridization State

Total number of	Nature of	Examples
sigma (σ) bonds	Hybridization State	
2	sp	BeCl <sub>2</sub> , HgCl <sub>2</sub> , C <sub>2</sub> H <sub>2</sub> , CO <sub>2</sub> , CO, CdCl <sub>2</sub> , ZnCl <sub>2</sub> etc.
3	sp <sup>2</sup>	BCl <sub>3</sub> , AlCl <sub>3</sub> , C <sub>2</sub> H <sub>4</sub> , C <sub>6</sub> H <sub>6</sub> , SO <sub>2</sub> , SO <sub>3</sub> , HNO <sub>3</sub> , H <sub>2</sub> CO <sub>3</sub> ,
		SnCl <sub>2</sub> , PbCl <sub>2</sub> etc.
4	sp <sup>3</sup>	NH4 <sup>+</sup> , BF4 <sup>-</sup> , H2SO4, HClO4, PCl3, NCl3, AsCl3,
		$\mathrm{HClO}_3,\mathrm{ICl}_2^+,\mathrm{OF}_2,\mathrm{HClO}_2,\mathrm{SCl}_2,\mathrm{HClO},\mathrm{ICl},\mathrm{XeO}_3$
		etc.
5	sp <sup>3</sup> d	PCl <sub>5</sub> , SbCl <sub>5</sub> , SF <sub>4</sub> , ClF <sub>3</sub> , BrF <sub>3</sub> , XeF <sub>2</sub> , ICl <sub>2</sub> <sup>-</sup> etc.
6	sp <sup>3</sup> d <sup>2</sup>	SF <sub>6</sub> , AlF <sub>6</sub> <sup>3-</sup> , SiF <sub>6</sub> <sup>2-</sup> , PF <sub>6</sub> <sup>-</sup> , IF <sub>5</sub> , BrF <sub>5</sub> , XeOF <sub>4</sub> , XeF <sub>4</sub> ,
		$BrF_4^-$ , $ICl_4^-$ etc.
7	sp <sup>3</sup> d <sup>3</sup>	IF <sub>7</sub> , XeF <sub>6</sub> etc.

## The geometry of simple molecules or ions

In absence of lone pair of electrons a molecule or ion exhibit regular geometry. For sp, sp<sup>2</sup>, sp<sup>3</sup>d, sp<sup>3</sup>d<sup>2</sup> and sp<sup>3</sup>d<sup>3</sup> hybridization state, geometry will be linear, trigonal planar, tetrahedral, trigonal bipyramid, octahedral and pentagonal bipyramid respectively, whereas for the same hybridization state in presence of the lone pair of electrons they exhibit subnormal geometry (see Figure 1, Table 2).



(Trigonal bipyramidal,  $sp^3d$ , LP=0) (Octahedral,  $sp^3d^2$ , LP=0) (Petntagonal bipyramidal,  $sp^3d^3$ , LP=0)



Hybridizatio	n LP	Molecular Geometry (Regular/Normal)	Approximate Bond Angles (Degree)	Examples	LP	Molecular Geometry (Sub-normal)	Approximate Bond Angles (Degree)	Examples
sp	0	Linear	180	$CO_2$ , $CS_2$ ,	-	-	-	-
				BeCl <sub>2</sub> , HgCl <sub>2</sub>				
sp <sup>2</sup>	0	Trigonal Planar	120	BH3, AlCl3,				
		or		$C_2H_4$ , $BCl_3$ ,	01	Angular or V-shape	<120	SO <sub>2</sub> , NO <sub>2</sub> -
		Triangular planar		BF3, NO3 <sup>-</sup> , CO3 <sup>2-</sup>				
sp <sup>3</sup>	0	Tetrahedral	109.5	BH4 <sup>-</sup> , BF4 <sup>-</sup> ,	01	Pyramidal	<109.5	NH3, PH3, AsH3
				SnCl <sub>4</sub> , H <sub>2</sub> SO <sub>4</sub>				
				HClO <sub>4</sub> , SiCl <sub>4</sub>				$H_2O$ , $H_2S$ , $H_2Se$
					02	Bent shape or V-shape	<109.5	
								ICl, BrF, ClF
					03	Linear	180	
sp³d	0	Trigonal	120	PF <sub>5</sub> , PCl <sub>5</sub>	01	See-Saw	<120(equatorial)	SF <sub>4</sub>
		bipyramid	(equatorial) 90				<90 (axial)	
			(axial)		02	T-shape	<90	ICl <sub>3</sub> ,F <sub>3</sub> Cl
					03	Linear	180	XeF2,I3 <sup>-</sup>
sp <sup>3</sup> d <sup>2</sup>	0	Octahedral	90	SF6, WF6, SeF6, SnCl6 <sup>2–</sup>	01	Square pyramidal	<90	IF5 <b>,</b> BrF5
					02	Square planar	90	XeF <sub>4</sub>
sp <sup>3</sup> d <sup>3</sup>	0	Pentagonal	72 <b>&amp;</b> 90	IF <sub>7</sub>		Pentagonal	72 & 90	
		bipyramid			01	Pyramidal or		$XeF_6$
						Distorted		
				octahedral				

Table 2. Hybridization, Molecular Geometry and Bond Angles without/with the lone pair of electrons

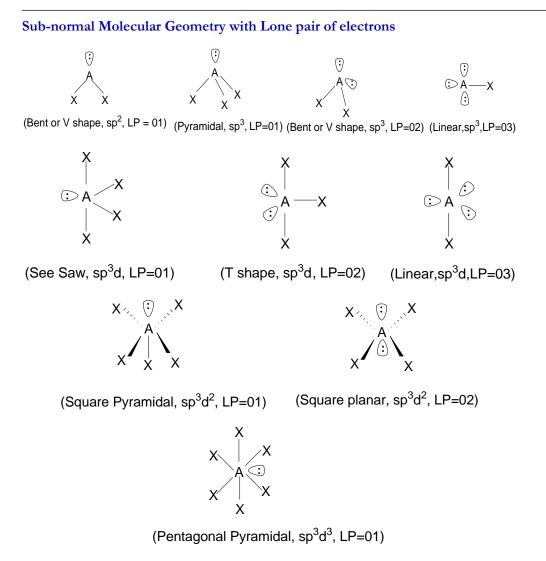


Figure 1. Pictorial diagram of the molecular geometry

## 2. Predicting the Hybridization of Heterocyclic Compounds

In this case, state of s-p hybridization of heteroatoms in heterocyclic compounds have been empirically calculated from the number of bonds and delocalized lone pair of electrons associated with it in the following way (Das, Paul, Sanjeev, and Jagannadham, 2014).

Total power on Hybridization State (X) = TNBS + DLP

Where, TNBS = Total Number of bonds directly attached with heteroatom excluding H bond if any attached with the hetero atom.

DLP = Delocalized lone pair electrons through resonance (Number of LP e-s on the heteroatom, which is directly attached to single bonds only).

- For sp; Power on s = 1 and Power on p = 1, Hence Total power = (1+1) = 2
- For  $sp^2$ ; Power on s = 1 and Power on p = 2, Hence Total power = 3 = (1+2) = 3
- For sp<sup>3</sup>; Power on s = 1 and Power on p = 3, Hence Total power = (1+3) = 4Examples are illustrated in Table-3.

Heterocyclic Compounds	TNBS (Total number of bonds around the hetero atom excluding H Bond)	DLP (Delocalized Lone Pair of e`s)	Total Power (X) = TNBS + DLP	Hybridization State
N N H Pyrrole	2	1	3	sp <sup>2</sup>
Ö. Furan	2	1 (out of two lone pairs of electrons, one can take part in delocalization at a time)	3	sp <sup>2</sup>
S. Thiophene	2	1 (out of two lone pairs of electrons, one can take part in delocalization at a time)	3	sp²
N. Pyridine	3	0 (lone pair on nitrogen does not undergo delocalization)	3	sp²
H Indole	2	1	3	sp²
Quinoline	3	0 (lone pair on nitrogen does not undergo delocalization)	3	sp <sup>2</sup>

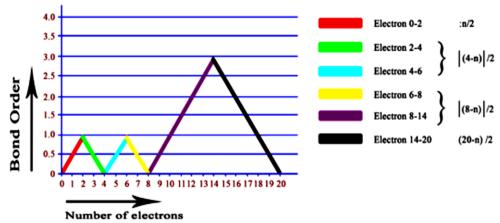
Table 3. Hybridization state of Heteroatoms in some Heterocyclic Compounds

# 3. Predicting the Bond-Order of Diatomic Species:

Bond-order usually predicted from the Molecular Orbital Theory. Molecular Orbital Theory (M.O.T.) was first proposed by Friedrich Hund and Robert Mulliken (Mulliken, R S., 1972; Hall, George G., 1991). They developed an approach to the covalent bond formation which is based upon the effects of the various electron fields upon each other and which employs molecular orbital rather than atomic orbital. Each such orbital characterizing the molecule as a whole is described by a definite combination of quantum numbers and possesses relative energy value.

## 3.1. For diatomic species having (1-20) e-s:

Graphical Representation of B.O. with the number of electrons



## BOND ORDER

Figure 2. B.O. vs number of electrons

The graphical representation presented in Figure 2 shows that bond-order gradually increases to 1 in the range (0-2) electrons then falls to zero in the range (2-4) electrons then it further rises to 1 for (4-6) electrons and once again falls to zero for (6-8) electrons then again rises to 3 in the range (8-14) electrons and then finally falls to zero for (14-20) electrons. For total no of electrons 2, 6 and 14, one can use multiple formulae, because they fall in the overlapping region in which they intersect with each other (Das, 2017).

First of all, I classify the molecules or ions into the following four (4) types based on the total number of electrons present in them.

i) Molecules and ions having total no of electrons within the range (1-2):

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

E.g. H<sub>2</sub> (Total e s = 2), therefore B.O. = n/2 = 2/2 = 1

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

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In such case Bond order = I 4 - n I / 2;

[where n = Total no of electrons, 'II' indicates Mod function i.e. the value of the bond order is always positive]

E. g.  $Li_2 + (5e-s)$  therefore B.O. = I 4 – 5 I / 2 = 1/2 = 0.5.

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

In such case Bond order = I 8 - n I / 2

E. g: CO (Total e s = 6+8=14), Therefore B.O. = I 8-14 I/2 = 3

iv) 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]

E.g. NO (Total e s = 15), therefore B.O. = 20 - 15/2 = 2.5

Bond order prediction with examples has been represented in Table-4.

Species	Total Number of e-s	Bond-Order		
(Molecules or ions)	(n)	(B.O.)		
Bond-Order Values for the species having (1-2) e <sup>-</sup> s; Bond order = $n/2$				
		-		
$H_2^+$	1	0.5		
H <sub>2</sub> , He <sub>2</sub> <sup>2+</sup>	2	1		
Bond-Order Values for th	ne species having (2-6) e	e's; Bond order = I 4- n I $/ 2$		
$H_2^-, He_2^+$	3	0.5		
He <sub>2</sub> ,	4	0		
Li <sub>2</sub> +,He <sub>2</sub> -	5	0.5		
Li <sub>2</sub> , He <sub>2</sub> <sup>2–</sup> , Be <sub>2</sub> <sup>2+</sup>	6	1		
Bond-Order Values for th	e species having (6-14)	e-s; Bond order = I 8- n I $/ 2$		
$Be_{2}^{+}, Li_{2}^{-}$	7	0.5		
Be <sub>2</sub> , Li <sub>2</sub> <sup>2–</sup>	8	0		
$Be_{2}^{-}, B_{2}^{+}$	9	0.5		
B <sub>2</sub> , Be <sub>2</sub> <sup>2-</sup> , HF	10	1		
B <sub>2</sub> -, C <sub>2</sub> +	11	1.5		
$C_2, B_2^{2-}, N_2^{2+}, CN^+$	12	2		
$C_2^-, N_2^+$	13	2.5		
N <sub>2</sub> , CO, NO <sup>+</sup> , C <sub>2</sub> <sup>2–</sup> , CN <sup>–</sup> , O <sub>2</sub> <sup>2+</sup>	14	3		
Bond-Order Values for th	e species having (14-20)	)e <sup>-</sup> s ; Bond order = (20-n) / 2		
N <sub>2</sub> <sup>-</sup> , NO, O <sub>2</sub> <sup>+</sup>	15	2.5		
$NO^{-}, O_{2}$	16	2		
O <sub>2</sub> -	17	1.5		
F <sub>2</sub> , O <sub>2</sub> <sup>2–</sup> , HCl	18	1		
$F_2^-$	19	0.5		
Ne <sub>2</sub>	20	0		

4. Predicting the Bond-Order of oxide-based acid radicals:

In case of oxide-based acid radicals

Charge on Acid Radical Total number of peripheral

atoms

Bond Order (B.O.) = Valency of the peripheral atom

E.g.:

 $ClO_4$ : (Valency of one Peripheral atom Oxygen = 2, Charge on acid radical = -1, Total Number of Peripheral atoms = 04), Therefore B.O. = 2 + (-1/4) = 1.75 $ClO_3$ : (Valency of one Peripheral atom Oxygen = 2, Charge on acid radical = -1, Total Number of Peripheral atoms = 03), Therefore B.O. = 2 + (-1/3) = 1.66 $ClO_2$ : (Valency of one Peripheral atom Oxygen = 2, Charge on acid radical = -1, Total Number of Peripheral atoms = 02), Therefore B.O. = 2 + (-1/2) = 1.5AsO $4^{3-}$ : (Valency of one Peripheral atom Oxygen = 2, Charge on acid radical = -3, Total Number of Peripheral atoms = 04), Therefore B.O. = 2 + (-3/4) = 1.25 $AsO_3^{3-}$ : (Valency of one Peripheral atom Oxygen = 2, Charge on acid radical = -3, Total Number of Peripheral atoms = 03), Therefore B.O. = 2 + (-3/3) = 1.0 $SO_4^2$ : (Valency of Peripheral atom Oxygen = 2, Charge on acid radical = -2, Number of Peripheral atoms = 04), Therefore B.O. = 2 + (-2/4) = 1.5 $SO_3^{2-}$ : (Valency of Peripheral atom Oxygen = 2, Charge on acid radical = -2, Number of Peripheral atoms = 03), Therefore B.O. = 2 + (-2/3) = 1.33 $PO_{4^{3-}}$ ; (Valency of Peripheral atom Oxygen = 2, Charge on acid radical = -3, Number of Peripheral atoms = 04), Therefore B.O. = 2 + (-3/4) = 1.25 $BO_{3^{3}}$ ; (Valency of Peripheral atom Oxygen = 2, Charge on acid radical = -3, Number of Peripheral atoms = 03), Therefore B.O. = 2 + (-3/3) = 1 $CO_3^{2-}$ ; (Valency of Peripheral atom Oxygen = 2, Charge on acid radical = -2, Number of Peripheral atoms = 03), Therefore B.O. = 2 + (-2/3) = 1.33 $SiO_4^{4-}$ : (Valency of Peripheral atom Oxygen = 2, Charge on acid radical = -4, Number of Peripheral atoms = 04), Therefore B.O. = 2 + (-4/4) = 1Relation of Bond order with Bond length, Bond Strength, Bond energy, Thermal stability and Reactivity:

B.O. α 1 / Bond length or Bond distance; B.O. α Bond strength; B.O. α Bond Energy;

B.O. α Thermal Stability; B.O. α 1 / Reactivity

Correlation among/between Literature values of bond-distances of some oxide based acid radicals with their predicted bond order values:

Literature values of the Cl-O average bond lengths in  $ClO_4^-$ ,  $ClO_3^-$  and  $ClO_2^-$ ; As-O bond lengths in  $AsO_4^{3-}$  and  $AsO_3^{3-}$  with respect to their bond order values suggest that with increasing bond-order M-O bond length (Where M = Cl, As etc.) decreases which is shown in Table 5.

Oxide Based Acid Radicals	Bond-Order Values	Avg. M-O Bond- Distances As per Literature (Å)	Remarks
ClO <sub>4</sub> -	1.75	1.50	
ClO3 <sup>-</sup>	1.6	1.57	Increasing Bond-
ClO <sub>2</sub> -	1.5	1.64	Order decreases
AsO4 <sup>3-</sup>	1.25	1.75	Bond Length
AsO3 <sup>3-</sup>	1.0	1.77	

 Table 5. Correlation of some bond-distances with their predicted bond order values

Correlation among/between Literature values of bond dissociation energy (KJ mol-1) of some molecules or ions with their predicted bond order values (Table-6).

Table 6. Correlation of some bond dissociation energy	gy with their predicted bond order values
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Molecules or ions	Bond-Order	Dissociation energy	Remarks
	Values	(KJ mol <sup>-1</sup> )	
$O_2^+$	2.5	642.9	Increasing Bond-
O <sub>2</sub>	2.0	493.6	Order increases
O <sub>2</sub> -	1.5	395.0	Bond dissociation
NO <sup>+</sup>	3.0	1046.9	energy (BDE)
NO	2.5	826.9	
NO-	2.0	487.8	

# 5. Magnetic Behavior of Diatomic Species

The present study involves three new formulae by just manipulating the number of unpaired electrons (n) using mod function (based on Applied Mathematics) and by means of these n values one can easily stumble the magnetic moment values in Bohr-Magneton using spin only formula  $\mu s = \sqrt{n(n+2)}$  B.M., where B.M. = Bohr Magneton = Unit of Magnetic Moment, n = number of unpaired electrons (Das, A., 2017).

First of all, we classify the molecules or ions depending on the total number of electrons present in them in the following three (03) sets.

Set-1: Molecules or ions having (1-3)e-s, (3-5)e-s, (5-7)e-s, (7-10)e-s, (13-16)e-s

Set-2: Molecules or ions having (10-13)e-s and (16-19)e-s

Set-3: Molecules or ions having 20 e-s

Then for the different set, we have to use three different formulae to calculate the number of unpaired electrons which have been presented in Table-7 and thus magnetic moment ( $\mu$ s in B.M.) can be evaluated in the following way:

5.1. F-1 (For Set-1) - for the determination of the number of unpaired electrons (n) of molecules or ions baving the total number of electrons (1-3), (3-5), (5-7), (7-10) and (13-16)e-s:

In this case, the number of unpaired electrons n = [I (ND - total e-s) I]

Here, ND = next digit i.e. digit next to minimum digit and 'II' indicates mod function.

E.g. Molecules or ions having (1-3)e-s, in this case, ND = 2 because here minimum digit is 1.

E.g. He<sub>2</sub>+ (3e-s), the total number of electrons will be 3, ND = 2, Hence, unpaired electron n = I (ND - total e-s) I = I (2-3) I = 1. Hence, Magnetic Moment  $\mu s = \sqrt{n(n+2)}$  B.M. =  $\sqrt{1(1+2)}$  BM =  $\sqrt{3}$  BM = 1.73BM.

For the molecules or ions containing (3-5)e-s, (5-7)e-s, (7-10)e-s, and (13-16)e-s the ND value will be 4, 6, 8 and 14 respectively.

Hence, the value of n = [ I (4-total e-s) I ]; [ I (6- total e-s) I ] [ I (8- total e-s) I ] and [ I (14- total e-s) I ] respectively.

5.2. F-2(For Set-2) - for the determination of the number of unpaired electrons (n) of molecules or ions having a total number of electrons (10-13) and (16-19):

In this case, the number of unpaired electrons n = [I (PD - total e-s) I]Here, PD = Penultimate electron digit (i.e. before last electron). Eg: for C<sub>2</sub>- (13e-s), the total number of electrons will be 13, PD = 12 Hence, unpaired electron n = I (12 - total e-s) I = I (12-13) I = 1Hence, Magnetic Moment  $\mu s = \sqrt{n(n+2)} B.M. = \sqrt{1(1+2)} BM = \sqrt{3} BM = 1.73BM$ For F<sub>2</sub> (18e-s), the total number of electrons will be 18, PD = 18 Hence, unpaired electron n = I (18 - total e-s) I = I (18-18) I = 0Hence, Magnetic Moment  $\mu s = \sqrt{n(n+2)} B.M. = \sqrt{0(0+2)} BM = 0 BM = Diamagnetic in nature.$ 

5.3. F-3 (For Set-3) - for the determination of number of unpaired electrons (n) of molecules or ions having total number of electrons 20:

In this case, the number of unpaired electrons n = [(20 - total e-s)]E.g. for Ne<sub>2</sub> (20e-s), the total number of electrons will be 20, Hence, unpaired electron n = (20 - total e-s) = (20-20) = 0Hence, Magnetic Moment  $\mu s = \sqrt{n(n+2)}$  B.M. =  $\sqrt{0(0+2)}$  BM = 0 BM = Diamagnetic in nature.

 $\uparrow$ 

#### Table 7. Magnetic moments of diatomic species

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Species	Total	Number of	Magnetic moment	Remark on
(Molecules or	Number	unpaired	(µs) in Bohr	magnetic
ions)	of e <sup>-</sup> s	electrons (n)	Magneton (B.M.)	behavior
$H_2^+$	1	1	1.73	Para magnetic
$H_2, He_2^{2+}$	2	0	0	Diamagnetic
H <sub>2</sub> <sup>-</sup> , He <sub>2</sub> <sup>+</sup>	3	1	1.73	Para magnetic
He <sub>2</sub>	4	0	0	Diamagnetic
Li <sub>2</sub> +, He <sub>2</sub> -	5	1	1.73	Para magnetic
Li <sub>2</sub> , He <sub>2</sub> <sup>2–</sup> , Be <sub>2</sub> <sup>2+</sup>	6	0	0	Diamagnetic
Be <sub>2</sub> <sup>+</sup> ,Li <sub>2</sub> <sup>-</sup>	7	1	1.73	Para magnetic
Be <sub>2</sub> , Li <sub>2</sub> <sup>2-</sup>	8	0	0	Diamagnetic
$Be_{2}^{-}, B_{2}^{+}$	9	1	1.73	Para magnetic
B <sub>2</sub> , Be <sub>2</sub> <sup>2-</sup> , HF	10	2	2.82	Para magnetic
B <sub>2</sub> -, C <sub>2</sub> +	11	1	1.73	Para magnetic
$C_2, B_2^{2-}, N_2^{2+}, CN^+$	12	0	0	Diamagnetic
C <sub>2</sub> -, N <sub>2</sub> +	13	1	1.73	Para magnetic
N <sub>2</sub> , CO, NO+,	14	0	0	Diamagnetic
$C_2^{2-}, CN^{-}, O_2^{2+}$				
N <sub>2</sub> -, NO, O <sub>2</sub> +	15	1	1.73	Para magnetic
NO <sup>-</sup> , O <sub>2</sub>	16	2	2.82	Para magnetic
O <sub>2</sub> -	17	1	1.73	Para magnetic
F2, O2 <sup>2</sup> , HCl	18	0	0	Diamagnetic
$F_2^-$	19	1	1.73	Para magnetic
Ne <sub>2</sub>	20	0	0	Diamagnetic

#### 6. Evaluating Spin Multiplicity

Spin-multiplicity value and its corresponding spin state were first discovered by Friedrich Hund in 1925. The formula which is generally used for the prediction of spin multiplicity value is [(2S+1), where  $S = \Sigma s =$  total spin quantum no] is time-consuming (Engel and Reid, 2006). To keep the matter in mind a simple innovative method has to be introduced for calculation of spin-multiplicity value and thus its corresponding spin state shown in Table-8, in the easiest way by ignoring the calculation of total spin quantum number ( $S = \Sigma s$ ) (Das, Sanjeev and Jagannadham, 2014).

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

## 6.1. Species having unpaired electrons in upward alignment (†):

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

${\leftarrow}$		

$\uparrow$	

Spin multiplicity = (n + 1) = (1+1) = 2 (spin state = doublet); (2+1) = 3 (spin state = triplet) and (3 + 1) = 4 (spin state = quartet) respectively.

$ \uparrow\downarrow\rangle \uparrow\uparrow  \uparrow\uparrow  \uparrow\uparrow  \uparrow\uparrow  \uparrow\uparrow  \uparrow\uparrow  \uparrow\uparrow  \uparrow\uparrow  \uparrow\uparrow $			$\uparrow \downarrow$	$\uparrow$	$\uparrow$	$\uparrow$	V	$\uparrow \downarrow$	$\uparrow$
--	--	--	-----------------------	------------	------------	------------	---	-----------------------	------------

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

# $\uparrow \downarrow \uparrow \downarrow \uparrow \downarrow$

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

6.2. Species having unpaired electrons in downward alignment  $(\downarrow)$ :

In this case spin multiplicity = (-n+1)

Here (-ve) sign indicate downward arrow.

$\downarrow$ $\downarrow$	$\downarrow$	$\downarrow$
---------------------------	--------------	--------------

Spin multiplicity = (-n + 1) = (-1 + 1) = 0; (-2 + 1) = -1 and (-3 + 1) = -2 respectively.

$\left  \downarrow \right  \downarrow \left  \downarrow \right  \qquad \left  \downarrow \right $	$\land \downarrow$	$\downarrow$	$\rightarrow$		↑↓
---	--------------------	--------------	---------------	--	----

Spin multiplicity = (-n + 1) = (-2 + 1) = -1 (ignore paired electrons) and (-1 + 1) = 0 respectively.

6.3. Species having unpaired electrons in both mixed alignment  $(\uparrow)$   $(\downarrow)$ :

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



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)

$$\uparrow \uparrow \downarrow$$

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

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

$$\uparrow \downarrow \uparrow \downarrow \uparrow$$

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 8. Spin multiplicity and corresponding Spin State

Number of unpaired electrons (n)	Spin multiplicity value $(n + 1)$	Spin state
0	1	Singlet
1	2	Doublet
2	3	Triplet
3	4	Quartet
4	5	Quintet
5	6	Multiplet

#### 7. Identifying Aromatic and Anti-Aromatic Compounds

It was first devised by Huckel in 1931 (Hückel, Erich, 1931; March, J., 1985). The present study will be an innovative method involving two formulae by just manipulating the number of  $\pi$  bonds within the ring system and delocalized electron pair (excluding  $\pi$  electron pair within the ring system) with one (01) (Das, A., Adhikari, S., Paul, B., Sanjeev, R. and Jagannadham, V. (2013); Das, A., Sanjeev, R. and Jagannadham, V., 2014).

#### 7.1. Prediction of Aromatic behavior:

In the first case, the compound must be cyclic, planar (i.e. all the carbon atoms having same state of hybridization) with even number of A value, where  $[A = \pi b + e - p + 1(constant)]$ , here  $\pi b =$  number of  $\pi$  bonds with in the ring system and e - p = number of electron pair outside or adjacent to the ring system i.e. if the ring contains hetero atoms (atoms containing lone pair of electrons) which can undergo delocalization and each negative charge if present may be treated as one pair of electrons.

If the value of 'A', for a certain organic compound comes out as an even number then this compound will be treated as aromatic compound.

#### 7.2. Prediction of Anti-aromatic behavior:

In the second case, the compound must be cyclic, planar (i.e. all the carbon atoms having the same state of hybridization) with odd number of A value, where  $[A = \pi b + e-p+1(constant)]$ , here  $\pi b$  = number of  $\pi$  bonds within the ring system and e-p = number of electron pair outside or adjacent to the ring system i.e. if the ring contains heteroatoms which can undergo delocalization and each negative charge if present, may be treated as one pair of electrons. If the value of 'A', for a certain organic compound comes out as an odd number then this compound will treat as an anti-aromatic compound.

7.3. General Condition for the Non-aromatic behavior of Organic Compounds:

Any compound that lacks one or more of the above features i.e. it may be acyclic / non-planar, is to be treated as nonaromatic. But in this case, 'A' value may be even or odd number. It is always to be noted that if the ring contains hetero atom like N, O, S etc, in this case, we must count that electron pair in the evaluation of 'A' value which can undergo delocalization. We never count localized electron pair. Examples have been illustrated in Table-9.

Table 9. Aromatic, anti-aromatic and non-aromatic behavior of organic compounds

	r		-	
Organic Compound (Cyclic, Planar/ Cyclic, non- planar)	$\pi b$ value [ $\pi b$ =number of $\pi$ bonds within the ring system]	ep value [ep = number of delocalized electron pair outside or adjacent to the ring system]	A value [A = πb + ep + 1 (constant)] (even no/ odd no)	Nature of compound (aromatic/ anti- aromatic/ non aromatic)
Benzene or [6] annulene (Cyclic, Planar)	$3 \pi$ bonds	0	3 + 0 + 1 = 4 (even no)	Aromatic
Naphthalene (Cyclic, Planar)	$5 \pi$ bonds	0	5 + 0 + 1 = 6 (even no)	Aromatic
Anthracene (Cyclic, Planar)	$7 \pi$ bonds	0	7 + 0 + 1 = 8 (even no)	Aromatic
Cyclopropene (Cyclic, non planar due to one sp <sup>3</sup> hybridized carbon atom)	$1 \pi$ bond	0	1 + 0 + 1 = 2 (even no)	Non-aromatic
Cyclopropenyl cation (Cyclic, Planar)	$1 \pi$ bond	0	1 + 0 + 1 = 2 (even no)	Aromatic
Cyclopropenyl anion (Cyclic, Planar)	$1 \pi$ bond	1 (For one negative charge on carbon which undergoes delocalization)	1 + 1+ 1 = 3 (odd no)	Anti-aromatic
Cyclobutadiene or [4] annulene (Cyclic, Planar)	$2 \pi$ bonds	0	2 + 0 + 1 = 3 (odd no)	Anti-aromatic
Cyclopentadiene (Cyclic, non planar due to one sp <sup>3</sup> hybridised carbon atom)	$2 \pi$ bonds	0	2 + 0 + 1 = 3 (odd no)	Non-aromatic
Cyclopentadienyl cation (Cyclic, Planar)	$2 \pi$ bonds	0	2 + 0 + 1 = 3 (odd no)	Anti-aromatic
Cyclopentadienyl anion (Cyclic, Planar)	$2 \pi$ bonds	01 (For one negative charge on carbon which undergo delocalization)	2 + 1 + 1 = 4 (even no)	Aromatic
Cyclooctatetraene or [8] annulene (Cyclic, Planar)	$4 \pi$ bonds	0	4 + 0 + 1 = 5 (odd no)	Anti-aromatic
Cyclooctatrienyl cation (Cyclic, non-planar due to one sp <sup>3</sup> hybridized carbon atom adjacent to positive charge)	$3 \pi$ bonds	0	3 + 0 + 1 = 4 (even no)	Non-aromatic
Pyridine (Cyclic, Planar)	$3 \pi$ bonds	0 (lone pair on N does not take part in delocalization)	3 + 0 + 1 = 4 (even no)	Aromatic
Pyrrole	$2 \pi$ bonds	1 (Here lone pair on N take part in delocalization)	2 + 1 + 1 = 4 (even no)	Aromatic
Furan	$2 \pi$ bonds	1 (Here out of two lone pairs on O only one LP take part in delocalization)	2 + 1 + 1 = 4 (even no)	Aromatic

There are some compounds which do not follow the above rule. Huckel's also cannot explain the aromatic or nonaromatic behavior of these compounds. These compounds have been represented in Table 10.

Organic Compound (Cyclic, Planar/ Cyclic, non-planar)	$\pi b$ value [ $\pi b$ =number of $\pi$ bonds within the ring system]	ep value [ep = number of delocalized electron pair outside or adjacent to the ring system]	A value [ $A = \pi b + ep + 1$ (constant)]	Nature of compound	$\pi b$ value [ $\pi b$ =number of $\pi$ bonds within the ring system]
1 HI 6	$5 \pi$ bonds	0	5 + 0 + 1 = 6 (even no.)	Not	Due to the interaction of the hydrogen of 1 and 6 compound become non-planar.
16	8 π bonds	0	8 + 0 + 1 = 9 (odd no.)	Aromatic	Because double bonded $C_{15}$ - $C_{16}$ do not take part in resonance.

Table 10. Omission behavior of aromatic and nonaromatic organic compounds

If we easily predict the nature of organic compound i.e. aromatic, anti-aromatic or nonaromatic then we can resolve different kind of problems regarding stability, reactivity, acidity etc. by using the following supposition.

1. Order of stability is aromatic > nonaromatic > anti-aromatic

2. Order of reactivity just follows the reverse order of stability as follows:

Anti-aromatic > non aromatic > aromatic

3. Acidity: Stability of Conjugate base  $\alpha$  acidity

E.g: cyclopentadienyl anion (aromatic) > cyclopentadiene (non-aromatic) > cyclopentadienyl cation (anti-aromatic). Hence, cyclopentadiene (its conjugate base i.e. Cyclopentadienyl anion is aromatic in nature) is much more acidic than cycloheptatriene (its conjugate base i.e. Cycloheptatrienyl anion is anti-aromatic in nature).

# 8. Calculating of $\pi$ -bonds, $\sigma$ -bonds, single and double bonds in Straight Chain and Cycloalkene Systems:

The molecular formula which defines a very large number of chemical structure, in this particular case, it is a herculean task to calculate the nature and number of bonds. Earlier, Badertscher et al studied a novel formalism to characterize the degree of unsaturation of organic molecules (Badertscher, M., Bischofberger, K., Munk, Morton E. and Pretsch, E., 2001). But no such work has not been taken till now to calculate the number and types of bonds in open chain olefinic

system having complex molecular formulae like C176H250, C2000H2000.

Keeping this in view, a rapid innovative method has been proposed for the calculation of the number of  $\pi$ -bonds,  $\sigma$ -bonds, single and double bonds with the help of following 06 (six) completely new formulae for certain aliphatic unsaturated open-chain and cyclic olefinic hydrocarbons (Das, A., Sanjeev, R. and Jagannadham, V., 2014).

## 8.1. For Open Chain Aliphatic Hydrocarbons

8.1.1. Calculation of  $\pi$ -bonds and double bonds (P): The number of  $\pi$  bonds or double bonds for a straight chain olefin is

P= [(2X-Y)/2] + 1, Where, X = number of carbon atoms; Y = number of hydrogen atoms and P = number of  $\pi$  bonds/double bonds. E.g.: In C176H250, X = 176, Y = 250, therefore P = (2 x 176 - 250)/2 + 1 = 51 + 1 = 52 number of  $\pi$  bonds or double bonds.

8.1.2. Calculation of  $\sigma$ -bonds (S):

The number of  $\sigma$  bonds for a straight chain olefin is S = [X + Y - 1]where, X = number of carbon atoms; Y = number of hydrogen atoms and S = number of sigma bonds ( $\sigma$ -bonds).

E.g.: In C176H250, X = 176, Y = 250, therefore  $P = 176 + 250 - 1 = 425 \sigma$  bonds.

8.1.3. Calculation of Single bonds (A):

The total number of single bond for a straight chain olefin is A = [(3Y/2)-2] where A = number of single bonds and Y is the number of hydrogen atoms.

E.g.: In C176H250, Y = 250, therefore A =  $[(3 \times 250)/2] = 375 - 2 = 373$  single bonds. Examples have been illustrated in Table-11.

Example (C <sub>x</sub> H <sub>y</sub> )	Straight-chain Structure	$\pi$ bond/ bonds [(2X-Y)/2+1]	σ bonds [X+Y-1]	Single bonds [(3Y/2)-2]	Double bond/bonds [(2X-Y)/2 + 1]
C <sub>2</sub> H <sub>4</sub>	H <sub>2</sub> C=CH <sub>2</sub>	1	5	4	1
C <sub>3</sub> H <sub>6</sub>	H <sub>2</sub> C=CH-CH <sub>3</sub>	1	8	7	1
C <sub>3</sub> H <sub>4</sub>	H <sub>2</sub> C=C=CH <sub>2</sub>	2	6	4	2
$C_4H_8$	i)H <sub>2</sub> C=CH-CH <sub>2</sub> -CH <sub>3</sub> ii)H <sub>3</sub> C-HC=CH-CH <sub>3</sub>	1	11	10	1
C <sub>4</sub> H <sub>6</sub>	i)H <sub>2</sub> C=C=CH-CH <sub>3</sub> ii)H <sub>2</sub> C=CH-CH=CH <sub>2</sub>	2	9	7	2
$C_4H_4$	$H_2C=C=C=CH_2$	3	7	4	3
$C_{176}H_{250}$	_	52	425	373	52
$C_{2000}H_{2000}$	-	1001	3999	2998	1001
C99H4	-	98	102	4	98

#### 8.2. For Cyclic aliphatic olefinic hydrocarbons:

#### 8.2.1. Calculation of $\pi$ -bonds and double bonds (Pc):

The number of  $\pi$  bonds or double bonds for an aliphatic cyclic olefin is Pc = [(2X-Y)/2], where, X = number of carbon atoms; Y = number of hydrogen atoms and Pc = number of  $\pi$  bonds or double bonds in the cyclic olefinic system.

E.g.: In cyclooctatetraene (C8H8),  $\dot{X} = Y = 8$ , therefore Pc = 16-8/2 = 4 number of  $\pi$  bonds or double bonds.

### 8.2.2. Calculation of $\sigma$ -bonds (Sc):

The number of  $\sigma$  bonds for an aliphatic cyclic olefin is Sc = [X + Y]

where X = number of carbon atoms; Y = number of hydrogen atoms and Sc = number of sigma bonds ( $\sigma$ -bonds) in a cyclic olefinic system.

E.g. In cyclooctatetraene (C8H8), X = Y = 8, therefore Sc = 8+8 = 16 number of  $\sigma$  bonds.

8.2.3. Calculation of Single bonds (Ac):

The total number of single bonds in aliphatic cyclic olefin can be calculated by using the formula Ac = [3Y/2] where Ac = number of single bonds and y is the number of hydrogen atoms in aliphatic cyclic olefin.

E.g.: In cyclooctatetraene (C8H8), Y = 8, therefore Ac = 24/2 = 12 number of single bonds. Examples have been illustrated in Table-12.

#### Table 12. Calculation of bonds in Cyclo Alkene system

Example (C <sub>x</sub> H <sub>y</sub> )	Cycloalkene	$\pi$ bond / bonds (P <sub>c</sub> ) = [(2X-Y)/2]	σ bonds (S <sub>c</sub> ) [X+Y]	Single bonds (A <sub>c</sub> ) [(3Y/2)]	Double bond/bonds [(2X-Y)/2]
$C_3H_4$	Cyclopropene	1	7	6	1
$C_4H_4$	Cyclobutadiene	2	8	6	2
$C_5H_6$	Cyclopentadiene	2	11	9	2
$C_6H_8$	Cyclohexadiene	2	14	12	2
$C_7H_8$	Cycloheptatriene	3	15	12	3
$C_8H_8$	Cyclooctatetraene	4	16	12	4

# 9. Calculation of $\pi$ -bonds, $\sigma$ -bonds, single and triple bonds in Straight Chain Alkyne And Cycloalkyne Systems:

The number and types of bonds in open chain and cycloalkynes having a complex molecular formula is a Herculean task. Keeping this in view, a rapid innovative method has been proposed for the calculation of number of  $\pi$ -bonds,  $\sigma$ -bonds, single and triple bonds with the help of following 08 (eight) completely new formulae by just manipulating the number of carbon and hydrogen atoms by using some factors for certain aliphatic unsaturated open chain and cycloalkynes (Das, Pal, Adhikari, Paul, Sanjeev, and Jagannadham, 2014; Das, Sanjeev and Jagannadham, 2014).

#### 9.1. Open Chain Aliphatic Alkynes

#### 9.1.1. Calculation of $\pi$ -bonds (P):

The number of  $\pi$  bonds for an aliphatic open chain alkyne, where there are one or more than one triple bonds is P= [{(2X-Y)/2} + 1], Where, X = number of carbon atoms; Y = number of hydrogen atoms and P = number of  $\pi$  bonds.

E.g.: In  $C_{16}H_{30}$ , X = 16, Y = 30,

therefore  $P = [\{(2X-Y)/2\} + 1] = [\{(2 \times 16 - 30)/2\} + 1] = 2$  number of  $\pi$  bonds.

9.1.2. Calculation of  $\sigma$ -bonds (S):

The number of  $\sigma$  bonds for an aliphatic open chain alkyne, where there are one or more than one triple bonds is S= [X+Y-1], Where, X = number of carbon atoms; Y = number of hydrogen atoms and S = number of  $\sigma$  bonds.

E.g.: In C<sub>16</sub>H<sub>30</sub>, X = 16, Y = 30, therefore, S= [X+Y-1] = [16+30-1] = 45 numbers of  $\sigma$  bonds. 9.1.3. Calculation of Single bonds (A):

The total number of single bond for an aliphatic open chain alkyne, where there are one or more than one triple bonds is  $A = [\{(2X+5Y)/2\} - 3]/2$ , Where, A = number of single bonds, X = number of carbon atoms and Y = number of hydrogen atoms.

E.g.: In C16H30, X = 16, Y = 30, therefore,  $A = [\{(2X+5Y) / 2\} - 3]/2$ 

 $= [\{(2x16+5x30)/2\}-3]/2 = [91-3]/2$ 

= 44 numbers of single bonds.

9.1.4. Calculation of Triple bonds (T):

In the first case, we have to count the number of carbon atoms (X) and the number of hydrogen atoms (Y) in a given unsaturated hydrocarbon containing triple bonds. The formula to calculate the number of triple bonds for an aliphatic open chain alkyne, where there are one or more than one triple bonds is

 $T = [{(2X-Y)/2} + 1]/2$ 

where, X = number of carbon atoms; Y = number of hydrogen atoms and T = number of triple bonds.

E.g.: In  $C_{16}H_{30}$ , X = 16, Y = 30, therefore,

T =  $[{(2X-Y)/2} + 1]/2 = [{(2 x 16 - 30)/2} + 1]/2 = 2/2 = 1$  triple bond. Examples have been illustrated in Table-13.

Example for Open Chain Alkyne (C <sub>x</sub> H <sub>y</sub> )	$\pi \text{ bonds} [\{(2X-Y)/2\} + 1]$	σ bonds [X+Y-1]	Single bonds [{(2X+5Y)/2} - 3]/2	Triple bond/bonds [{(2X-Y)/2} + 1]/2
C10H18	2	27	26	1
C11H20	2	30	29	1
$C_{12}H_{22}$	2	33	32	1
C13H24	2	36	35	1
$C_{14}H_{26}$	2	39	38	1
C15H28	2	42	41	1
C16H30	2	45	44	1
$C_6H_6$	4	11	9	2
C <sub>12</sub> H <sub>14</sub>	6	25	22	3

#### Table 13. Calculation of bonds in open chain Alkyne system

#### 9.2. Cycloalkynes:

#### 9.2.1. Calculation of $\pi$ -bonds (Pc):

In the first case, we have to count the number of carbon atoms (X) and the number of hydrogen atoms (Y) in the given unsaturated cycloalkyne. The formula to calculate the number of  $\pi$  bonds for an aliphatic cycloalkyne is

Pc = [(2X-Y)/2]

where X = number of carbon atoms; Y = number of hydrogen atoms and Pc = number of  $\pi$  bonds in the cycloalkyne system.

E.g.: In Cycloheptyne (C7H10), X =7, Y = 10, therefore Pc = (2x7-10)/2 = 2 number of  $\pi$  bonds. 9.2.2. Calculation of  $\sigma$ -bonds (Sc):

The number of  $\sigma$  bonds for an aliphatic cycloalkyne is Sc = [X + Y]

where, X = number of carbon atoms; Y = number of hydrogen atoms and Sc = number of sigma bonds ( $\sigma$ -bonds) in cyclo alkyne system.

E.g.: In Cycloheptyne (C7H10), X =7, Y = 10, therefore Sc = (7+10) = 17 number of  $\sigma$  bonds.

#### 9.2.3. Calculation of Single bonds (Ac):

The total number of single bond for an aliphatic cycloalkyne is  $Ac = [\{(2X+5Y)/2\}]/2$ ; where, Ac = number of single bonds in cycloalkyne, X = number of carbon atoms and Y = number of hydrogen atoms.

E.g.: In Cycloheptyne (C7H10), X = 7, Y = 10,

therefore, Ac =  $[{(2X+5Y)/2}]/2 = [{(2x7+5x10)/2}]/2=32/2 = 16$  numbers of single bonds. 9.2.4. Calculation of Triple bonds (T):

The number of triple bond is  $Tc = [{(2X-Y)/2}]/2$ 

where, X = number of carbon atoms; Y = number of hydrogen atoms and Tc = number of triple bond.

E.g.: In Cycloheptyne (C7H10), X =7, Y = 10, therefore, Tc =  $[\{(2X-Y)/2\}]/2 = [\{(2 \ge 7 - 10)/2\}]/2 = 2/2 = 1$  triple bond.

#### Conclusions

It may be expected that these time economic innovative mnemonics would go a long way to help the students of chemistry at Undergraduate, Senior Undergraduate and Post-Graduate level who would choose the subject as their career. Experiment in vitro on 100 students showed that by using these formulae students can save up to 30-40 mins time in the examination hall. On the basis of this, I can strongly recommend using these time economic innovative mnemonics in the field of chemical education.

#### Acknowledgment

I am grateful to the SERB, DST, New Delhi, Govt. of India, for their financial assistance (Sanction no – SERB / F / 5537 / 2013-14 dated 27/11/2013 and D.O. No. SB / EMEQ - 014 / 2013).

I want to delegate my this innovative review article in the field of Chemical Education to my father Late Anil Ranjan Das, who was also a chemistry teacher and also founder of my chemistry. Furthermore, I want to give my cordial honor and gratitude to the newly elected Honorable Chief Minister of 'Tripura', Mr.Biplab Kumar Deb and Honorable Education & Higher Education Minister of Tripura, Mr.Ratan Lal Nath for their constant valuable sustaining mentality to improve our state in all respect.

In addition to these, I give my special accolade to Prof.M.K.Singh, Dean of Science, Tripura University, Tripura, India; Mr. Sanit Debroy, Registrar, Tripura University, Tripura, India and Mr.Sekhar Datta, Senior Journalist 'The Telegraph' for their constant valuable sustaining mentality to carry out the my innovational research work in the field of chemical education.

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