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.

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, 2013; Das, Pal, Adhikari, Paul, 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_4) 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, sp², sp³ 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) - sp² hybrid orbital;

s + p (1:3) - sp³ hybrid orbital

A formula used for the determination of sp, sp², and sp³ hybridization state:

$$\left(\begin{array}{c} \text{Power on the Hybridization} \\ \text{state of the central atom} \end{array} \right) = \left(\begin{array}{c} \text{Total no of σ bonds} \\ \text{around each central atom} \end{array} \right) - 1$$

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

This translates into the following:

a. In NH_3: central atom N is surrounded by three N-H single bonds i.e. three sigma (σ) bonds and one lone pair (LP) i.e. one additional σ bond. So, in NH_3 there is a total of four σ 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 = sp³.

b. In H_2O: central atom O is surrounded by two O-H single bonds i.e. two sigma (σ) bonds and two lone pairs i.e. two additional σ bonds. So, all together in H_2O, there are four σ 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_2O = sp^3.

c. In H_3BO_3:- B has 3σ bonds (3BPs but no LPs) and oxygen has 4σ bonds (2BPs & 2LPs) so, in this case, power of the hybridization state of B = 3-1 = 2 i.e. B is sp^2 hybridized in H_3BO_3. On the other hand, the power of the hybridization state of O = 4-1= 3 i.e. hybridization state of O in H_3BO_3 is sp^3.
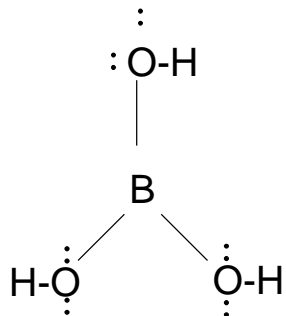
d. In I-Cl: I and Cl both have 4σ bonds and 3LPs, so, in this case, power of the hybridization state of both I and Cl=4−1=3 i.e. hybridization state of I and Cl both are sp^3.

e. In $CH_2=CH_2$: each carbon is attached with 2 C-H single bonds (2 σ bonds) and one C=C bond (1σ 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^2.
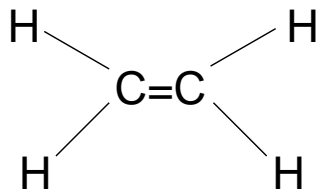
1.2. *Prediction of sp^3d, sp^3d^2, sp^3d^3 Hybridization state:*

In case of sp^3d, sp^3d^2 and sp^3d^3 hybridization state there is a common term sp^3 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:-
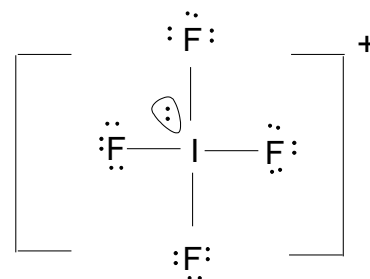
5σ bonds = 4σ bonds + 1 additional σ bond = sp^3d hybridization

6σ bonds = 4σ bonds + 2 additional σ bonds = sp^3d^2 hybridization

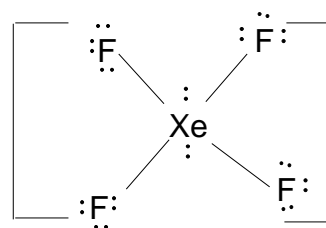7σ bonds = 4σ bonds + 3 additional σ bonds = sp^3d^3 hybridization
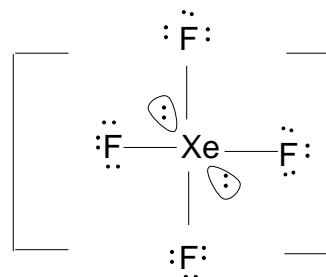
This translates into the following:

a. IF_4^+:

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 σ bonds. So, 5σ bonds = 4 σ bonds + 1 additional σ bond = sp^3d hybridization

b. XeF_4:

Lewis Structure of XeF_4:

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 σ bonds = 04 σ bonds + 02 additional σ bonds = sp^3d^2 hybridization.

c. IF_7: 7 I-F single bonds i.e. 7σ bonds = 4σ bonds + 3 additional σ 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. σ bonds and corresponding hybridization State

Total number of sigma (σ) bonds	Nature of Hybridization State	Examples
2	sp	$BeCl_2$, $HgCl_2$, C_2H_2, CO_2, CO, $CdCl_2$, $ZnCl_2$ etc.
3	sp^2	BCl_3, $AlCl_3$, C_2H_4, C_6H_6, SO_2, SO_3, HNO_3, H_2CO_3, $SnCl_2$, $PbCl_2$ etc.
4	sp^3	NH_4^+, BF_4^-, H_2SO_4, $HClO_4$, PCl_3, NCl_3, $AsCl_3$, $HClO_3$, ICl_2^+, OF_2, $HClO_2$, SCl_2, HClO, ICl, XeO_3 etc.
5	sp^3d	PCl_5, $SbCl_5$, SF_4, ClF_3, BrF_3, XeF_2, ICl_2^- etc.
6	sp^3d^2	SF_6, AlF_6^{3-}, SiF_6^{2-}, PF_6^-, IF_5, BrF_5, $XeOF_4$, XeF_4, BrF_4^-, ICl_4^- etc.
7	sp^3d^3	IF_7, XeF_6 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^2, sp^3, sp^3d, sp^3d^2 and sp^3d^3 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).

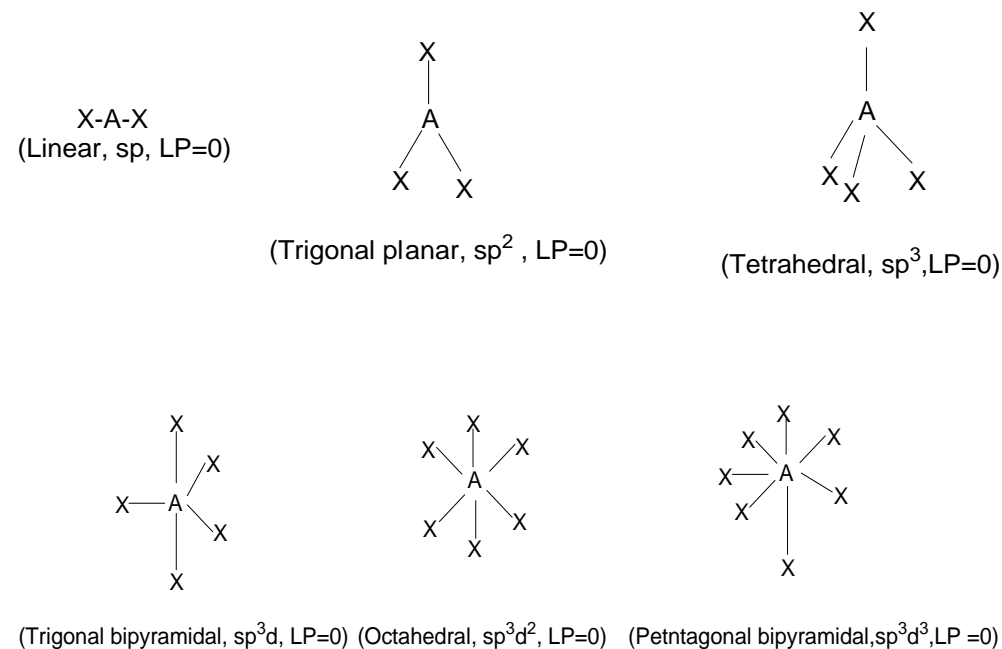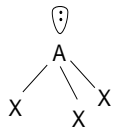**Regular/Normal Molecular Geometry without Lone pair of electrons**

X-A-X
(Linear, sp, LP=0)

(Trigonal planar, sp^2, LP=0)

(Tetrahedral, sp^3, LP=0)

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

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

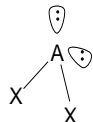| Hybridization	LP	Molecular Geometry (Regular/Normal)	Approximate Bond Angles (Degree)	Examples	LP	Molecular Geometry (Sub-normal)	Approximate Bond Angles (Degree)	Examples
sp	0	Linear	180	CO_2, CS_2, $BeCl_2$, $HgCl_2$	-	-	-	-
sp^2	0	Trigonal Planar or Triangular planar	120	BH_3, $AlCl_3$, C_2H_4, BCl_3, BF_3, NO_3^-, CO_3^{2-}	01	Angular or V-shape	<120	SO_2, NO_2^-
sp^3	0	Tetrahedral	109.5	BH_4^-, BF_4^-, $SnCl_4$, H_2SO_4 $HClO_4$, $SiCl_4$	01	Pyramidal	<109.5	NH_3, PH_3, AsH_3 H_2O, H_2S, H_2Se
					02	Bent shape or V-shape	<109.5	ICl, BrF, ClF
					03	Linear	180	
sp^3d	0	Trigonal bipyramid	120 (equatorial) 90 (axial)	PF_5, PCl_5	01	See-Saw	<120(equatorial) <90 (axial)	SF_4
					02	T-shape	<90	ICl_3, F_3Cl
					03	Linear	180	XeF_2, I_3^-
sp^3d^2	0	Octahedral	90	SF_6, WF_6, SeF_6, $SnCl_6^{2-}$	01	Square pyramidal	<90	IF_5, BrF_5
					02	Square planar	90	XeF_4
sp^3d^3	0	Pentagonal bipyramid	72 & 90	IF_7	01	Pentagonal Pyramidal or Distorted octahedral	72 & 90	XeF_6

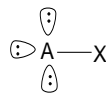## Sub-normal Molecular Geometry with Lone pair of electrons
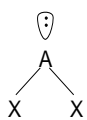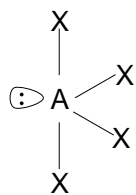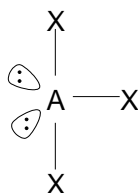

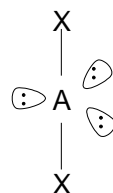(Bent or V shape, sp², LP = 01)   (Pyramidal, sp³, LP=01)   (Bent or V shape, sp³, LP=02)   (Linear,sp³,LP=03)
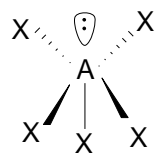
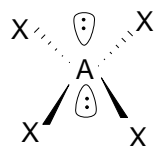(See Saw, sp³d, LP=01)   (T shape, sp³d, LP=02)   (Linear,sp³d,LP=03)
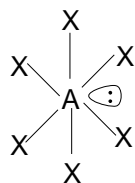
(Square Pyramidal, sp³d², LP=01)   (Square planar, sp³d², LP=02)

(Pentagonal Pyramidal, sp³d³, LP=01)

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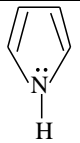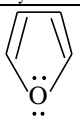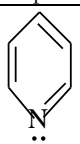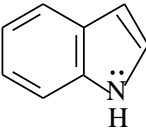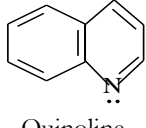
DLP = Delocalized lone pair electrons through resonance (Number of LP e-s on the heteroatom, which is directly attached to single bonds only).

- For sp; Power on s = 1 and Power on p = 1, Hence Total power = (1+1) = 2
- For sp²; Power on s =1 and Power on p = 2, Hence Total power = 3 = (1+2) = 3
- For sp³; Power on s = 1 and Power on p = 3, Hence Total power = (1+3) = 4

Examples are illustrated in Table-3.

Figure 1. Pictorial diagram of the molecular geometry

Table 3. Hybridization state of Heteroatoms in some Heterocyclic Compounds

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
Pyrrole	2	1	3	sp^2
Furan	2	1 (out of two lone pairs of electrons, one can take part in delocalization at a time)	3	sp^2
Thiophene	2	1 (out of two lone pairs of electrons, one can take part in delocalization at a time)	3	sp^2
Pyridine	3	0 (lone pair on nitrogen does not undergo delocalization)	3	sp^2
Indole	2	1	3	sp^2
Quinoline	3	0 (lone pair on nitrogen does not undergo delocalization)	3	sp^2

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
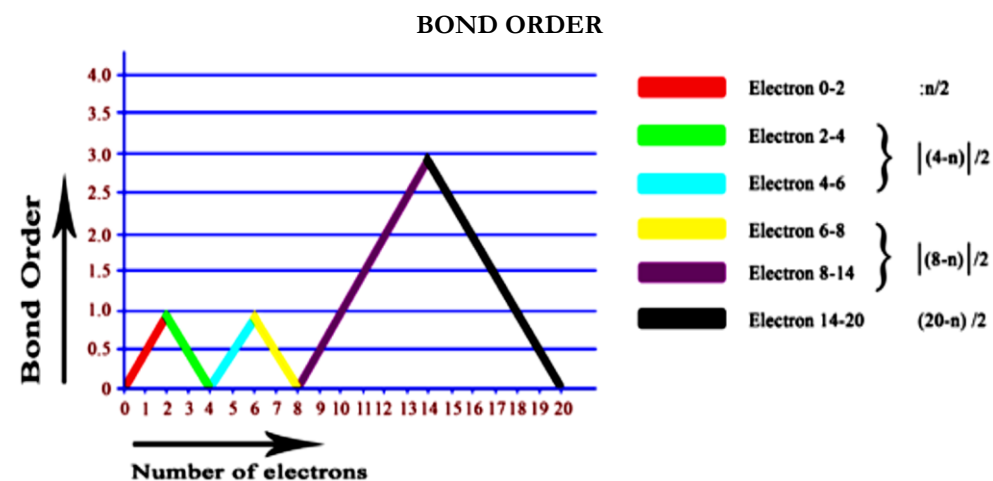
BOND ORDER

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_2 (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):

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

[where n = Total no of electrons, 'I' 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.

Table 4. Bond order values of diatomic species having (1-20) e-s

Species (Molecules or ions)	Total Number of e-s (n)	Bond-Order (B.O.)
Bond-Order Values for the species having (1-2) e-s; Bond order = n/2		
H_2^+	1	0.5
H_2, He_2^{2+}	2	1
Bond-Order Values for the species having (2-6) e-s; Bond order = I 4- n I / 2		
H_2^-,He_2^+	3	0.5
He_2,	4	0
Li_2^+,He_2^-	5	0.5
Li_2, He_2^{2-}, Be_2^{2+}	6	1
Bond-Order Values for the species having (6-14) e-s; Bond order = I 8- n I / 2		
Be_2^+, Li_2^-	7	0.5
Be_2, Li_2^{2-}	8	0
Be_2^-, B_2^+	9	0.5
B_2, Be_2^{2-}, HF	10	1
B_2^-, C_2^+	11	1.5
C_2, B_2^{2-}, N_2^{2+}, CN^+	12	2
C_2^-, N_2^+	13	2.5
N_2, CO, NO^+, C_2^{2-}, CN^-, O_2^{2+}	14	3
Bond-Order Values for the species having (14-20)e-s ; Bond order = (20-n) / 2		
N_2^-, NO, O_2^+	15	2.5
NO^-, O_2	16	2
O_2^-	17	1.5
F_2, O_2^{2-}, HCl	18	1
F_2^-	19	0.5
Ne_2	20	0

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

In case of oxide-based acid radicals

$$Bond\ Order\ (B.O.) = Valency\ of\ the\ peripheral\ atom + \frac{Charge\ on\ Acid\ Radical}{Total\ number\ of\ peripheral\ atoms}$$

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) = 1.5

$AsO4^{3-}$: (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) = 1

Relation 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.

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

Oxide Based Acid Radicals	Bond-Order Values	Avg. M-O Bond-Distances As per Literature (Å)	Remarks
ClO_4^-	1.75	1.50	Increasing Bond-Order decreases Bond Length
ClO_3^-	1.6	1.57	
ClO_2^-	1.5	1.64	
AsO_4^{3-}	1.25	1.75	
AsO_3^{3-}	1.0	1.77	

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 with their predicted bond order values

Molecules or ions	Bond-Order Values	Dissociation energy (KJ mol^{-1})	Remarks
O_2^+	2.5	642.9	Increasing Bond-Order increases Bond dissociation energy (BDE)
O_2	2.0	493.6	
O_2^-	1.5	395.0	
NO^+	3.0	1046.9	
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 (µs 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 having 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_2^+ (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 µs = $\sqrt{n(n+2)}$ 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_2^- (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 = 1
Hence, Magnetic Moment µs = $\sqrt{n(n+2)}$ B.M. = $\sqrt{1(1+2)}$ BM = $\sqrt{3}$ BM = 1.73BM
For F_2 (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 = 0
Hence, Magnetic Moment µs = $\sqrt{n(n+2)}$ 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_2 (20e-s), the total number of electrons will be 20,
Hence, unpaired electron n = (20 - total e-s) = (20-20) = 0
Hence, Magnetic Moment µs = $\sqrt{n(n+2)}$ B.M. = $\sqrt{0(0+2)}$ BM = 0 BM = Diamagnetic in nature.

Table 7. Magnetic moments of diatomic species

| Species (Molecules or ions)	Total Number of e⁻s	Number of unpaired electrons (n)	Magnetic moment (μ_s) in Bohr Magneton (B.M.)	Remark on magnetic behavior
H_2^+	1	1	1.73	Para magnetic
H_2, He_2^{2+}	2	0	0	Diamagnetic
H_2^-, He_2^+	3	1	1.73	Para magnetic
He_2	4	0	0	Diamagnetic
Li_2^+, He_2^-	5	1	1.73	Para magnetic
Li_2, He_2^{2-}, Be_2^{2+}	6	0	0	Diamagnetic
Be_2^+, Li_2^-	7	1	1.73	Para magnetic
Be_2, Li_2^{2-}	8	0	0	Diamagnetic
Be_2^-, B_2^+	9	1	1.73	Para magnetic
B_2, Be_2^{2-}, HF	10	2	2.82	Para magnetic
B_2^-, C_2^+	11	1	1.73	Para magnetic
C_2, B_2^{2-}, N_2^{2+}, CN^+	12	0	0	Diamagnetic
C_2^-, N_2^+	13	1	1.73	Para magnetic
N_2, CO, NO^+, C_2^{2-}, CN^-, O_2^{2+}	14	0	0	Diamagnetic
N_2^-, NO, O_2^+	15	1	1.73	Para magnetic
NO^-, O_2	16	2	2.82	Para magnetic
O_2^-	17	1	1.73	Para magnetic
F_2, O_2^{2-}, HCl	18	0	0	Diamagnetic
F_2^-	19	1	1.73	Para magnetic
Ne_2	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 = Σs = 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 = Σs) (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 (↑):

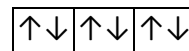In this case, spin multiplicity = (n+1); where n = number of unpaired electrons
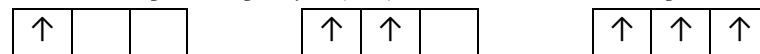
Spin multiplicity = (n +1) = (1+1) = 2 (spin state = doublet); (2+1) = 3 (spin state = triplet) and (3 + 1) = 4 (spin state = quartet) respectively.

Spin multiplicity = (n +1) = (2 + 1) = 3 (in this case ignore paired electrons) (spin state = triplet) and (1 + 1) = 2 (spin state = doublet)
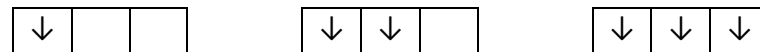
Spin multiplicity = (n +1) = (0 + 1) = 1 (spin state = singlet)

6.2. Species having unpaired electrons in downward alignment (↓):

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

Here (-ve) sign indicate downward arrow.

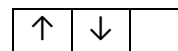Spin multiplicity = (–n +1) = (–1 + 1) = 0; (–2 + 1) = -1 and (–3 + 1) = -2 respectively.

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 (↑) (↓):

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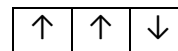
Here the total no of unpaired electrons = 3 in which two unpaired electrons lie in upward (+2) and one unpaired electron lie in downward (–1).

Hence Spin multiplicity = [(+n) + (–n) + 1] = [(+2) + (–1) + 1] = 2 (spin state = doublet)
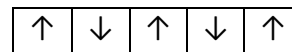
Here the total no of unpaired electrons = 5 in which three unpaired electrons lie upward (+3) and two unpaired electrons lie downward (–2).

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 π bonds within the ring system and delocalized electron pair (excluding π 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 = πb+e-p+1(constant)], here πb = number of π 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 = πb+e-p+1(constant)], here πb = number of π 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.

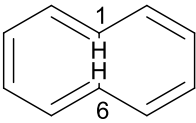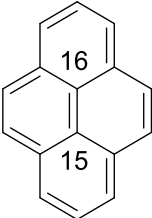### 7.3. General Condition for the Non-aromatic behavior of Organic Compounds:

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

Organic Compound (Cyclic, Planar/ Cyclic, non-planar)	πb value [πb =number of π bonds within the ring system]	e-p value [e-p = number of delocalized electron pair outside or adjacent to the ring system]	A value [A = πb + e-p + 1 (constant)] (even no/ odd no)	Nature of compound (aromatic/ anti-aromatic/ non aromatic)
Benzene or [6] annulene (Cyclic, Planar)	3 π bonds	0	3 + 0+1 = 4 (even no)	Aromatic
Naphthalene (Cyclic, Planar)	5 π bonds	0	5 + 0 +1 = 6 (even no)	Aromatic
Anthracene (Cyclic, Planar)	7 π bonds	0	7 + 0 + 1 = 8 (even no)	Aromatic
Cyclopropene (Cyclic, non planar due to one sp³ hybridized carbon atom)	1 π bond	0	1 + 0 + 1 = 2 (even no)	Non-aromatic
Cyclopropenyl cation (Cyclic, Planar)	1 π bond	0	1 + 0 + 1 = 2 (even no)	Aromatic
Cyclopropenyl anion (Cyclic, Planar)	1 π 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 π bonds	0	2 + 0 + 1 = 3 (odd no)	Anti-aromatic
Cyclopentadiene (Cyclic, non planar due to one sp³ hybridised carbon atom)	2 π bonds	0	2 + 0 + 1 = 3 (odd no)	Non-aromatic
Cyclopentadienyl cation (Cyclic, Planar)	2 π bonds	0	2 + 0 + 1 = 3 (odd no)	Anti-aromatic
Cyclopentadienyl anion (Cyclic, Planar)	2 π 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 π bonds	0	4 + 0 + 1 = 5 (odd no)	Anti-aromatic
Cyclooctatrienyl cation (Cyclic, non-planar due to one sp³ hybridized carbon atom adjacent to positive charge)	3 π bonds	0	3 + 0 + 1 = 4 (even no)	Non-aromatic
Pyridine (Cyclic, Planar)	3 π bonds	0 (lone pair on N does not take part in delocalization)	3 + 0 + 1 = 4 (even no)	Aromatic
Pyrrole	2 π bonds	1 (Here lone pair on N take part in delocalization)	2 + 1 + 1 = 4 (even no)	Aromatic
Furan	2 π 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.

Table 10. Omission behavior of aromatic and nonaromatic organic compounds

Organic Compound (Cyclic, Planar/ Cyclic, non-planar)	πb value [πb =number of π 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)]	Nature of compound	πb value [πb =number of π bonds within the ring system]
	5 π bonds	0	5 + 0 + 1 = 6 (even no.)	Not aromatic	Due to the interaction of the hydrogen of 1 and 6 compound become non-planar.
	8 π bonds	0	8 + 0 + 1 = 9 (odd no.)	Aromatic	Because double bonded C$_{15}$-C$_{16}$ do not take part in resonance.

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 α 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 π-bonds, σ-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 π-bonds, σ-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 π-bonds and double bonds (P): The number of π 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 π bonds/double bonds. E.g.: In C176H250, X = 176, Y = 250, therefore P = (2 x 176 – 250)/2 +1 = 51 + 1 = 52 number of π bonds or double bonds.

8.1.2. Calculation of σ-bonds (S):

The number of σ 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 (σ-bonds).
E.g.: In C176H250, X = 176, Y = 250, therefore P = 176 + 250 -1 = 425 σ 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 x 250)/2] = 375 -2 = 373 single bonds. Examples have been illustrated in Table-11.

Table 11. Calculation of bonds in open chain olefinic hydrocarbons

Example (C$_x$H$_y$)	Straight-chain Structure	π bond/ bonds [(2X-Y)/2+1]	σ bonds [X+Y-1]	Single bonds [(3Y/2)-2]	Double bond/bonds [(2X-Y)/2 + 1]
C$_2$H$_4$	H$_2$C=CH$_2$	1	5	4	1
C$_3$H$_6$	H$_2$C=CH-CH$_3$	1	8	7	1
C$_3$H$_4$	H$_2$C=C=CH$_2$	2	6	4	2
C$_4$H$_8$	i)H$_2$C=CH-CH$_2$-CH$_3$ ii)H$_3$C-HC=CH-CH$_3$	1	11	10	1
C$_4$H$_6$	i)H$_2$C=C=CH-CH$_3$ ii)H$_2$C=CH-CH=CH$_2$	2	9	7	2
C$_4$H$_4$	H$_2$C=C=C=CH$_2$	3	7	4	3
C$_{176}$H$_{250}$	-	52	425	373	52
C$_{2000}$H$_{2000}$	-	1001	3999	2998	1001
C$_{99}$H$_4$	-	98	102	4	98

8.2. For Cyclic aliphatic olefinic hydrocarbons:

8.2.1. Calculation of π-bonds and double bonds (Pc):

The number of π 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 π bonds or double bonds in the cyclic olefinic system.

E.g.: In cyclooctatraene (C8H8), X = Y = 8, therefore Pc = 16-8/2 = 4 number of π bonds or double bonds.

8.2.2. Calculation of σ-bonds (Sc):

The number of σ 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 (σ-bonds) in a cyclic olefinic system.

E.g: In cyclooctatetraene (C8H8), X = Y = 8, therefore Sc = 8+8 = 16 number of σ 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_xH_y)	Cycloalkene	π bond / bonds (P_c) = $[(2X-Y)/2]$	σ bonds (S_c) $[X+Y]$	Single bonds (A_c) $[(3Y/2)]$	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 π-bonds, σ-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 π-bonds, σ-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 π-bonds (P):

The number of π 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 π 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 π bonds.

9.1.2. Calculation of σ-bonds (S):

The number of σ 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 σ bonds.

E.g.: In $C_{16}H_{30}$, X = 16, Y = 30, therefore, $S = [X+Y-1] = [16+30-1] = 45$ numbers of σ 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, $A = [\{(2X+5Y) / 2\} - 3]/2$

$$= [\{(2 \times 16+5 \times 30)/2\}-3]/2 = [91-3]/2$$

$$= 44 \text{ numbers of single bonds.}$$

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,

$T = [\{(2X-Y)/2\} + 1]/2 = [\{(2 \times 16 - 30)/2\} +1]/2 = 2/2 = 1$ triple bond.

Examples have been illustrated in Table-13.

Table 13. Calculation of bonds in open chain Alkyne system

Example for Open Chain Alkyne (C_xH_y)	π 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
$C_{10}H_{18}$	2	27	26	1
$C_{11}H_{20}$	2	30	29	1
$C_{12}H_{22}$	2	33	32	1
$C_{13}H_{24}$	2	36	35	1
$C_{14}H_{26}$	2	39	38	1
$C_{15}H_{28}$	2	42	41	1
$C_{16}H_{30}$	2	45	44	1
C_6H_6	4	11	9	2
$C_{12}H_{14}$	6	25	22	3

9.2. Cycloalkynes:

9.2.1. Calculation of π-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 π 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 π bonds in the cycloalkyne system.

E.g.: In Cycloheptyne (C7H10), X =7, Y = 10, therefore Pc = (2x7-10)/2 = 2 number of π bonds.

9.2.2. Calculation of σ-bonds (Sc):

The number of σ 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 (σ-bonds) in cyclo alkyne system.

E.g.: In Cycloheptyne (C7H10), X =7, Y = 10, therefore Sc = (7+10) = 17 number of σ 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 x 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.

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References

Badertscher, M., Bischofberger, K., Munk, Morton E. and Pretsch, E. (2001). A Novel Formalism To Characterize the Degree of Unsaturation of Organic Molecules. *J. Chem. Inf. Comput. Sci. 41*(4), 889-893. (Retrieved from: https://pubs.acs.org/doi/abs/10.1021/ci000135o)

Cotton, F.A., Wilkinson G. and Gaus, P.L. (2007). *Basic Inorganic Chemistry*. Wiley: India, 3rd ed., 107, 523, 111.

Das, A., Paul, B., Sanjeev, R. and Jagannadham, V. (2014). Time Economic Innovative Methodology on the Prediction of Hybridization State of Heterocyclic Compounds. IOSR *Journal of Applied Chemistry, 7*(8 II), 38-39, doi: 10.9790/5736-07412429 (Retrieved from: http://www.iosrjournals.org/iosr-jac/papers/vol7-issue8/Version-2/G07823839.pdf)

Das, A., (2017). Bond-order and Magnetic Behavior of Diatomic Species without Molecular Orbital Theory. World *Journal of Chemical Education. 5*(4), 128-131, doi: 10.12691/wjce-5-4-2. (Retrieved from: http://www.sciepub.com/WJCE/abstract/7659)

Das, A., Adhikari, S., Paul, B., Sanjeev, R. and Jagannadham, V. (2013). A rapid and innovative method for the identification of aromatic and anti-aromatic nature of organic compounds. *World Journal of Chemical Education, 1*(1), 6-8, doi: 10.12691/wjce-1-1-2. (Retrieved from: http://www.sciepub.com/WJCE/abstract/632)

Das, A., Pal, D., Adhikari, S., Paul, B., Sanjeev, R. and Jagannadham, V. (2014). Rapid calculation of the number of π-bonds, σ-bonds, single and triple bonds in aliphatic Unsaturated open chain and cycloalkynes. *World Journal of*

Chemical   Education,   2(1),   1-3,   doi:10.12691/wjce-2-1-1.   (Retrieved   from:
     http://www.sciepub.com/WJCE/abstract/1268)

Das, A., Sanjeev, R. and Jagannadham, V. (2014). Innovative And Time Economic Pedagogical Views In Chemical
     Education - A Review Article. *World Journal of Chemical Education, 2*(3), 29-38, doi:10.12691/wjce-2-3-1 (Retrieved
     from: http://pubs.sciepub.com/wjce/2/3/1/index.html)

Douglas, B., Mcdaniel, D. and Alexander, J. (2007). *Concepts and Models of Inorganic Chemistry.* Wiley: India, 3rd ed., 157, 38.

Engel, T. and Reid, P. (2006). *Physical Chemistry.Pearson Benjamin-Cummings*, 473, 477–479, ISBN 080533842X. (Retrieved
     from: https://en.wikipedia.org/wiki/Hund%27s_rule_of_maximum_multiplicity#cite_ref-2)

Finar, I. L. (2004). *Organic Chemistry.* Vol-1, Pearson, 6th ed., 1, 532, 577-580.

Finar, I. L. (2002). *Organic Chemistry.* Vol-2, Pearson, 5th ed., 606-637, ISBN: 81-7808-164-4.

Hall, G. G. (1991). The Lennard-Jones Paper of 1929 and the foundations of Molecular Orbital Theory. *Advances in
     Quantum   Chemistry.   22*,   1-6.   doi: 10.1016/S0065-3276(08)60361-5.   (Retrieved   from:
     https://www.sciencedirect.com/science/article/pii/S0065327608603615?via%3Dihub)

Hückel, E. (1931).Quantentheoretische Beiträge zum Benzolproblem I. Die Elektronenkonfiguration des Benzols und
     verwandter Verbindungen. *Z. Phys. 70* (3–4), 204–86. Bibcode: 1931ZPhy...70..204H. doi:10.1007/BF01339530.
     (Retrieved from: https://link.springer.com/article/10.1007%2FBF01339530)

Lee, J. D. (2009). *Concise Inorganic Chemistry.* Wiley: India and Oxford, 5th ed., 944, 109-112.

Mahan B. M. and Meyers, R. J. (1998). *International Student Edition University Chemistry*. 4th ed., 599-603.

March, J. (1985). *Advanced Organic Chemistry: Reaction, Mechanisms and Structure.* Willy: New York, 3rd ed., ISBN 0-471-
     85472-7.

Morrison, R. T. and Boyd, R.N. (1999). *Organic Chemistry. Pearson*, 7th ed. 208.

Mulliken, R. S. (1972*). Spectroscopy, Molecular Orbitals, and Chemical Bonding. Nobel Lectures, Chemistry 1963-1970.* Amsterdam:
     Elsevier (Retrieved from: https://www.nobelprize.org/nobel_prizes/chemistry/laureates/1966/mulliken-
     lecture.html)

Pauling, L. (1931). The Nature Chemical Bond. Application of Results Obtained from the Quantum Mechanics and from
     a Theory of Paramagnetic Susceptibility to the Structure of Molecules. *J. Am. Chem. Soc., 53*(4), 1367-1400,
     doi:10.1021/ja01355a027.(Retrieved from: https://pubs.acs.org/doi/abs/10.1021/ja01355a027)

Smith, J. G. (2008). *Organic Chemistry.* 2nd ed., 616-619.

Solomons T. W. Graham and Fryhle, C. B. (2012). *Organic Chemistry.* Wiley: India 10th ed., 632-639.

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