INNOVATIVE MNEMONICS IN CHEMICAL EDUCATION: REVIEW ARTICLE

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ABSTRACT

In this review article, formulae based innovative mnemonics have been discussed to create interest and remove phobia of students in the field of chemical education. Educators can use these numerous mnemonics in their teaching style in the classroom lectures after discussing conventional methods to make chemistry intriguing. Here, I have tried to focus some time economic mnemonics by including thirty-three (33) new formulae in the field of chemical education. It will encourage students to solve multiple choice type questions (MCQs) at different competitive examinations in a time economic ground. This review article emphasizes chemical education in the light of a variety of mnemonic techniques to make it metabolic, time economic and intriguing for students because the use of mnemonics in classroom lectures is an essential tool to become a distinguished educator. *[African Journal of Chemical Education—AJCE 8(2), July 2018]*

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 including heterocyclic compounds, evaluation of magnetic behavior 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 [1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16,17,18,19].

Keeping this in mind, in this pedagogical review article, I have introduced some innovative mnemonic techniques to make chemistry metabolic, time economic and interesting [20,21,22,23,24,25,26,27]. Here, I have tried to discuss them abruptly.

METHODOLOGY

2.1. Innovative mnemonics for predicting hybridization state of simple molecules or ions:

Hybridization state theory

Prof. Pauling (1931), first developed the Hybridization state theory in order to explain the structure of molecules such as methane (CH_4) using atomic orbitals [1, 2]. This concept was developed for simple chemical systems but this one applied more widely later on and from today's point of view it is considered an operative empirical for excusing the structures of organic and inorganic compounds along with their related problems.

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

2.1.1. *Prediction of sp, sp^2, sp^3 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^2 hybrid orbital ;

s + p (1:3) - sp^3 hybrid orbital

Formula: prediction of sp, sp^2, and sp^3 hybridization state

Power on the Hybridization state of the central atom (P_{Hyb}) = (T_{SLP}) – 1

where, P_{Hyb} = Power on the Hybridization state of the central atom,

T_{SLP} = (Total no of σ bonds around each central atom + LP)

From the Lewis structure of a molecule, first of all, predict the number of sigma bonds (σ-bonds), pi bonds (π-bonds) and the lone pair of electrons (LP) 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 Co-ordinate bond (→) can be treated as 1σ bond. This formula is applicable up to four (04) T_{SLP}. If the power of the hybridization state (P_{Hyb}) will be 03, 02 and 01 then the hybridization state will be sp^3, sp^2 and sp respectively [21, 24, 26].

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 four (04) T_{SLP} is responsible. So, with four (04) T_{SLP}, for each additional T_{SLP} (additional sigma bond or lone pair of electron), added one d orbital gradually as follows: -

$$\mathbf{5\ T_{SLP} = 4\ T_{SLP} + 1\ additional\ T_{SLP} = sp^3d\ hybridization}$$

$$\mathbf{6\ T_{SLP} = 4\ T_{SLP} + 2\ additional\ T_{SLP} = sp^3d^2\ hybridization}$$

$$\mathbf{7\ T_{SLP} = 4\ T_{SLP} + 3\ additional\ T_{SLP} = sp^3d^3\ hybridization}$$

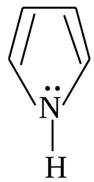
In case of cationic species, requisite electron/electrons must be removed from the outermost orbit of the central atom and in case of anionic species, added requisite electron with the outermost electrons of the central atom [21, 24, 26].

2.2. Innovative mnemonic for Predicting hybridization state of hetero atom in different heterocyclic compounds:

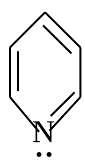
Classification of Lone Pair of Electrons in heterocyclic compounds

Lone Pair of electrons can be generally classified into two types as Delocalized lone pair of electron (DLP) and Localized lone pair of electron (LLP) as follows:

i)Delocalized lone pair of electron (DLP): When lone pair of electron of hetero atom undergo delocalization through conjugation then it is to be treated as delocalized lone pair of electron (DLP). Hetero atom (atom containing lone pair of electron) which is directly attached with single bonds only from all ends is to be considered as DLP containing hetero atom and its lone pair is to be treated as (DLP).

Eg. In Pyrrole  lone pair of N atom is to be treated as DLP because it is directly attached with three single bonds only.

ii)*Localized lone pair of electron (LLP)*: When lone pair of electron of hetero atom does not undergo delocalization through conjugation then it is to be treated as Localized lone pair of electron (LLP). Hetero atom (atom containing lone pair of electron) which is directly attached with single and double bonds with the ring system is to be considered as LLP containing hetero atom and its lone pair is to be treated as localized lone pair of electron (LLP).

Eg. In Pyridine  lone pair of N atom is to be treated as LLP because it is directly attached with double and single bonds with the ring system.

Planarity of Heterocyclic Compounds

Planarity is one of the vital features for prediction aromatic, anti-aromatic and non-aromatic behavior of heterocyclic compounds or other organic compounds. For aromatic and anti-aromatic behavior, the compound must be planar, whereas, non-planar compound is non aromatic in nature [12,13,14,15,16,17,18]. Planarity of heterocyclic compounds depends on the nature of the hybridization state of carbon and hetero atoms present in it. When all atoms (carbon and hetero) in the heterocyclic compounds having sp^2 hybridized then it is planar but when there is a mixing of sp^2 and sp^3 hybridization state then it is treated as non-planar.

2.2.1. *Prediction of sp^2 and sp^3 Hybridization state*

Formula: prediction of sp^2 and sp^3 hybridization state

Power on the Hybridization state of the hetero atom (P_{Hyb}) = (T_{SLLP}) – 1

where, P_{Hyb} = Power on the Hybridization state of the hetero atom, T_{SLLP} = (Total no of σ bonds around each central atom + LLP), LLP = Localized lone pair of electron.

If the power of the hybridization state (P_{Hyb}) will be 03, 02 and 01 then the hybridization state will be sp^3, sp^2 and sp respectively. All single (-) bonds are σ bond, in double bond (=) there is one σ and one π. In addition to these each localized lone pair of electron (LLP) can be treated as one σ bond [27].

2.2. 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 in 1933 [3, 4]. They developed an approach to 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.

First of all, classify the molecules or ions having (1-20)e-s into the following four (4) types based on total number of electrons present in them [21, 24, 25, 26].

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

In such case Bond order = n/2

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

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

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

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

2.2.4. 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, ‘I I’ indicates Mod function i.e. the value of bond order is always positive]

2.3. Prediction of Bond-Order of oxide based acid radicals:

Bond order of oxide based acid radicals can be calculated from the simple molecular formulae of the acid radicals in the following way [21, 24, 26].

In case of oxide based acid radicals

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

= 2 + (Charge on Acid Radical / Total number of peripheral atoms)

2.4. Prediction 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 [21, 24, 25, 26].

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 different set we have to use three different formulae to calculate the number of unpaired electrons and thus magnetic moment (μ_s in B.M.) can be evaluated in the following way:

2.4.1. F-1(For Set-1) - for the determination of number of unpaired electrons (n) of molecules or ions having 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 ‘I I’ indicates mod function.

Eg: Molecules or ions having (1-3)e^{-}s, in this case ND = 2 because here minimum digit is 1.

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.

2.4.2. F-2 (For Set-2) - for the determination of number of unpaired electrons (n) of molecules or ions having 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).

For the molecules or ions containing (10-13) and (16-19)e^{-}s the PD value will be 12 and 18 respectively.

Hence, the value of n = [I (12 - total e^{-}s) I] and [I (18 - total e^{-}s) I] respectively.

2.4.3. 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)]

2.5. Evaluating Spin Multiplicity

Spin-multiplicity value and its corresponding spin state was 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 [6]. 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 in the easiest way by ignoring the calculation of total spin quantum number (S = Σs).

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 [21, 24, 26]**.**

2.5.1. Species having unpaired electrons in upward alignment (↑):

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

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

In this case **spin multiplicity = (-n+1)**; Here (-ve) sign indicate downward arrow.

2.5.3. 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.

2.6. Innovative Mnemonics for Identifying Aromatic and Anti-Aromatic Organic Compounds

It was first devised by Huckel in 1931 [12,13,14,15,16,17,18]. 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) [20, 21, 24].

Conventional methods:

Aromatic nature of organic compound

1. Cyclic molecule,

2. Planer molecule in which all bonded atoms lie in same plane (having sp^2 hybridized)

3. Conjugated molecule with conjugated π-electron system,

4. Contains (4n + 2) π electrons, where, n is a positive integer (n = 0,1,2,3 etc.)

Anti-Aromatic nature of organic Compound:

1. Cyclic molecule,
2. Planer molecule in which all bonded atoms lie in same plane (having sp^2 hybridized)
3. Conjugated molecule with conjugated π-electron system,
4. 4nπ electrons, where, n is a positive integer (n = 0,1,2,3 etc.)

Non Aromatic Nature of organic Compound:

If a compound violates any one of the above three conditions (1 or 2 or 3) then it is non aromatic in nature.

2.6.1. 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) and conjugated 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 even number then this compound will be treated as aromatic compound.

2.6.2. Prediction of Anti-aromatic behavior:

In the second case, the compound must be cyclic, planar (i.e. all the carbon atoms having same state of hybridization) and conjugated with **odd 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 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 odd number then this compound will treat as anti-aromatic compound.

2.6.3. General Condition for 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 non-aromatic. 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.

2.7. Innovative Mnemonics for the Prediction of Aromatic, Anti Aromatic behavior of Heterocyclic Compounds with DLP:

The present study will be an innovative mnemonic involving calculation of 'A' value by just manipulating the no of π bonds within the ring system and delocalized lone pair of electron (DLP) with one (01) [27].

The heterocyclic compound having cyclic, planar, conjugated (i.e. all the carbon atoms having same state of hybridization, sp^2) with even number of 'A' value will be treated as aromatic in nature and with odd number of 'A' value will be treated as anti-aromatic in nature.

Formula: **Evaluation of A Value to predict Aromatic and Anti Aromatic Nature**

A = πb+DLP+1(constant) = even no = Aromatic

A = πb+DLP+1(constant) = odd no = Anti Aromatic

where, πb = number of π bonds with in the ring system;

DLP = Delocalized lone pair of electron.

In case of a multi hetero atom based heterocyclic compound, containing both DLP and LLP hetero atoms, Aromatic and Anti Aromatic behavior should be predicted with respect to DLP based hetero atom only. But when heterocyclic compounds contain both LLP based hetero atoms then Aromaticity should be predicted with respect to that hetero atom which contains lowest possible position number as per IUPAC nomenclature or any one of the hetero atom.

2.8. 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 [19]. 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 $C_{176}H_{250}$, $C_{2000}H_{2000}$.

Keeping this in view, a rapid innovative method has been proposed for the calculation of 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 [21, 23, 24].

2.8.1. For Open Chain Aliphatic Hydrocarbons

(i) 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.

(ii) 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).

(iii) 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 number of hydrogen atoms.

2.8.2. For Cyclic aliphatic olefinic hydrocarbons

(i) Calculation of π-bonds and double bonds (P_c):

The number of π bonds or double bonds for an aliphatic cyclic olefin is **P_c= [(2X-Y)/2];** Where, X = number of carbon atoms; Y = number of hydrogen atoms and P_c = number of π bonds or double bonds in the cyclic olefinic system.

(ii) Calculation of σ-bonds (S_c):

The number of σ bonds for an aliphatic cyclic olefin is **S_c = [X + Y];** Where, X = number of carbon atoms; Y = number of hydrogen atoms and S_c = number of sigma bonds (σ-bonds) in cyclic olefinic system.

(iii) Calculation of Single bonds (A_c):

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

2.9. 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 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 [21, 22, 24].

2.9.1. Open Chain Aliphatic Alkynes

(i) Calculation of π-bonds (P):

The number of π bonds for an aliphatic open chain alkyne, where there is 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.

(ii)Calculation of σ-bonds (S):

The number of σ bonds for an aliphatic open chain alkyne, where there is 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.

(iii)Calculation of Single bonds (A):

The total number of single bond for an aliphatic open chain alkyne, where there is 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.

(iv)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 is 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.

2.9.2. Cycloalkynes

(i) Calculation of π-bonds (P_c):

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 $\mathbf{P_c = [(2X-Y)/2]}$; where, X = number of carbon atoms; Y = number of hydrogen atoms and P_c = number of π bonds in the cycloalkyne system.

(ii) Calculation of σ-bonds (S_c):

The number of σ bonds for an aliphatic cycloalkyne is $\mathbf{S_c = [X + Y]}$; where, X = number of carbon atoms; Y = number of hydrogen atoms and S_c = number of sigma bonds (σ-bonds) in cycloalkyne system.

(iii) Calculation of Single bonds (A_c):

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

(iv) Calculation of Triple bonds (T):

The number of triple bond is $\mathbf{T_c = [\{(2X-Y)/2\}]/2}$; where, X = number of carbon atoms; Y = number of hydrogen atoms and T_c = number of triple bond.

RESULTS AND DISCUSSION

Prediction of the hybridization state (sp, sp^2 & sp^3) of simple molecules and ions can be well explained in the following way

Eg.:

a) NH_3: In NH_3, central atom N is surrounded by three N-H single bonds i.e. three (03) sigma (σ) bonds and one (01) lone pair (LP). So, T_{SLP} = 4, in NH_3, hence, power on the hybridization state of N in NH_3, $(P_{Hyb}) = (T_{SLP}) – 1= (3+1)-1 = 3$ i.e. hybridization state = sp^3.

b) H_2O: In H_2O, central atom O is surrounded by two O-H single bonds i.e. two (02) sigma (σ) bonds and two (02) lone pairs. So, in this case, power on the hybridization state of O, $(P_{Hyb}) = (T_{SLP}) – 1= = (2+2)-1 = 3$, i.e. hybridization state of O in H_2O = sp^3.

c) H_3BO_3:- In H_3BO_3, B has **(Fig.1)**, three (03) σ bonds only (no LPs) and oxygen has two (02) σ bonds and two (02) lone pair of electrons, so, in this case, power on the hybridization state of B, $(P_{Hyb}) = (T_{SLP}) – 1= (3+0)-1 = 2$ i.e. B is sp^2 hybridized in H_3BO_3. On the other hand, the power of the hybridization state of O, $(P_{Hyb}) = (T_{SLP}) – 1= = (2+2)-1= 3$ i.e. hybridization state of O in H_3BO_3 is sp^3.

d) I-Cl: In I-Cl, I and Cl both have one (01) σ bond and three (03) lone pair of electrons, so, in this case, power on the hybridization state of both I and Cl, $(P_{Hyb}) = (T_{SLP}) – 1= (1+3) - 1 = 3$ i.e. hybridization state of I and Cl both are sp^3.

e) $CH_2 = CH_2$: In C_2H_4, each carbon **(Fig.1)**, is attached with two (02) C-H single bonds (2 σ bonds) and one C=C bond (1σ bond), so, altogether there are 3 sigma bonds. So, in this case, the power on the hybridization state of both C, $(P_{Hyb}) = (T_{SLP}) – 1= (3+0)-1 = 2$ i.e. hybridization state of both carbons are sp^2.

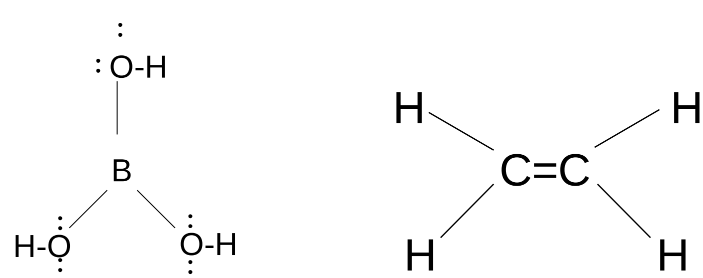


Fig. 1 Structure of H_3BO_3 and C_2H_4

f) O_3: Ozone (O_3) exists as a stable form of cyclic ozone **(Fig.2)** and its structure is equilateral triangle [2, 5]. In which each center O atom has two (02) O-O single bonds (2σ bonds) and two (02) lone pair of electrons. So, in this case, power on the hybridization state of central O atom (P_{Hyb}) = (T_{SLP}) – 1= (2+2) - 1 = 3 i.e. hybridization state of center atom O in cyclic O_3 is sp^3.

But the resonance description of ozone involves two structures **(Fig.3)**, in which, central oxygen atom of ozone will have sp^2 hybridization state. In this case, the central O atom has two (02) σ bonds and one (01) lone pair of electron (LP = 01), hence, power on the hybridization state of central O atom in resonance hybrid of ozone, (P_{Hyb}) = (T_{SLP}) – 1= (2+1) - 1 = 2 (sp^2).

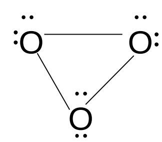


Fig. 2 Equilateral triangle structure of cyclic ozone (O_3)

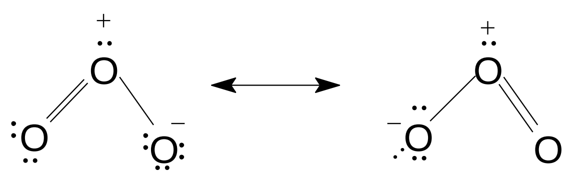


Fig. 3 Resonating structures of Ozone (O_3)

g) S_8: The ordinary form of sulfur (orthorhombic sulfur, yellow crystals) contains octatomic molecules (S_8), in which, S can form single covalent bonds with two other S atoms in a zigzag fashion **(Fig.4)**, into a long chain. In this case, each sulfur atom attached with two (02) adjacent σ bonds and two (02) lone pair of electrons (LP = 2). Hence, power on the hybridization state of any S atom (P_{Hyb}) = (T_{SLP}) – 1= (2+2) - 1 = 3 i.e. hybridization state of S atoms in S_8 is sp^3.

h) P_4: In P_4, the four P atoms are arranged at the corners of a regular tetrahedron **(Fig.4)**. Here, each P atom forms three covalent bonds (3σ bonds) and one lone pair of electron (LP = 1).

Hence, power on the hybridization state of any P atom (P_{Hyb}) = (T_{SLP}) – 1= (3+1) - 1 = 3 i.e. hybridization state of P atoms in P_4 is sp^3.

(S_8) **(P_4)**

Fig. 4 Zigzag structure of S_8 and Tetrahedron structure of P_4

i) CO_3^{2-} : In the valence bond structure of carbonate ion (CO_3^{2-}), the central carbon atom does not contain any lone pair of electron (LP = 0) but it has three (03) σ bonds **(Fig.5)**. Hence, power on the hybridization state of central C atom in carbonate ion, (P_{Hyb}) = (T_{SLP}) – 1= (3+0) - 1 = 2 (sp^2). But in resonance hybrid of CO_3^{2-} **(Fig.6)**, carbon atoms are in sp^2 hybridization state due to 3 σ bonds and no lone pair of electrons (LP = 0).

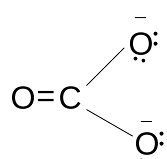


Fig. 5 Valence bond structure of carbonate ion (CO_3^{2-})

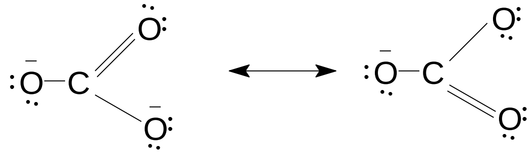


Fig. 6 Resonance hybrid of CO_3^{2-}

Prediction of the hybridization state (sp^3d, sp^3d^2 & sp^3d^3) of simple molecules and ions can be well explained in the following way

Eg:-

a) I_3^-: In Tri iodide ion (I_3^-), central I atom has 2σ bonds and 3 lone pair of electrons (LP = 3) **(Fig.7)**. Hence for central I, there is 5 T_{SLP} So, 5 T_{SLP} = 4 T_{SLP} + 1 additional T_{SLP} = sp^3d hybridization.

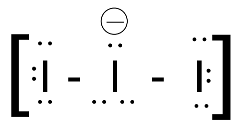


Fig. 7 Linear structure of tri iodide ion (I_3^-)

b) IF_4^+: In IF_4^+ **(Fig.8)**, 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 four (04) I-F σ bonds and there is one (01) LP. So, altogether there are 5 T_{SLP}. So, 5 T_{SLP} = 4 T_{SLP} + 1 additional T_{SLP} = sp^3d hybridization.

c) XeF_4: In XeF_4 **(Fig.8)**, Xe, an inert gas, consider 8 e^-s in its outermost shell, four (04) of which form four (04) Xe-F sigma bonds and there are two (02) lone pair of electrons, so, altogether there is 06 T_{SLP} = 4 T_{SLP} + 2 additional T_{SLP} = sp^3d^2 hybridization.

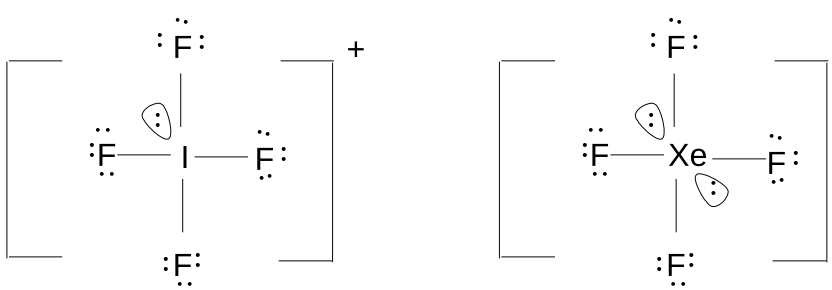


Fig. 8 Structure of IF_4^+ and XeF_4

a) IF_7: In IF_7, there is seven (07) I-F single bonds i.e. 7σ bonds and no lone pair of electron (LP), so, altogether there is 07 T_{SLP} = 4 T_{SLP} + 3 additional T_{SLP} = sp^3d^3 hybridization.

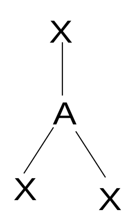
In case of determination of the hybridization state by using the above method, one must have a clear idea about the outermost electrons of different family members in the periodic table as follows:

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

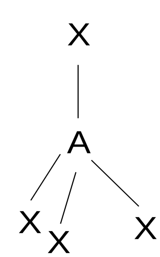
The geometry of simple molecules or ions

In absence of lone pair of electrons (LPs) a molecule or ion exhibit regular geometry (Fig.9). 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 (Fig.10) [8, 9, 10].

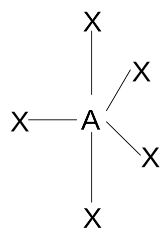
X-A-X
(Linear, sp, LP=0)



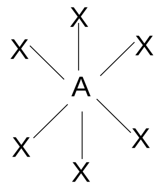
(Trigonal planar, sp^2 , LP=0)



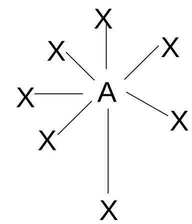
(Tetrahedral, sp^3,LP=0)



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

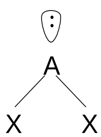


(Octahedral, sp^3d^2, LP=0)

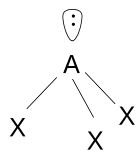


(Petntagonal bipyramidal,sp^3d^3,LP =0)

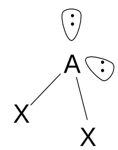
Fig.9 Regular / Normal Molecular Geometry without Lone pair of electrons



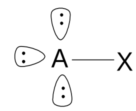
(Bent or V shape, sp^2, LP = 01)



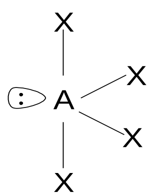
(Pyramidal, sp^3, LP=01)



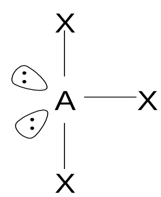
(Bent or V shape, sp^3, LP=02)



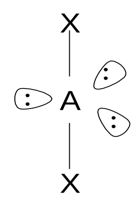
(Linear,sp^3,LP=03)



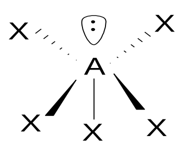
(See Saw, sp^3d, LP=01)



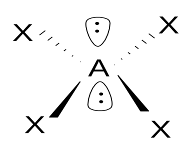
(T shape, sp^3d, LP=02)



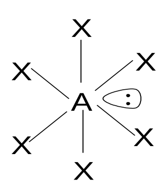
(Linear,sp^3d,LP=03)



(Square Pyramidal, sp^3d^2, LP=01)



(Square planar, sp^3d^2, LP=02)



(Pentagonal Pyramidal, sp^3d^3, LP=01)

Fig. 10 Sub-normal Molecular Geometry with Lone pair of electrons

Prediction of the hybridization state (sp^2 & sp^3) of* hetero atom in heterocyclic compounds *can be well explained in the following way

Hybridization state of hetero atom in heterocyclic compounds can be calculated from the total number of σ bonds around hetero atom and number of localized lone pair of electrons (T_{SLLP}) on the hetero atom and subtract one (01) from this total value of T_{SLLP} to get the hybridization state (sp^2 & sp^3) of the hetero atom in the heterocyclic compounds.

Adequate examples on prediction of the hybridization state from the corresponding T_{SLP} value (total number of σ bonds around the central atom + lone pair of electron on central atom) of the central atom have been explored in Table 1. Molecular Geometry (normal and sub normal) and bond angle with respect to the corresponding hybridization state and lone pair of electrons of simple molecules or ions have been displayed in Table 2. Hybridization state of hetero atom in heterocyclic compounds containing one, two or more same or different number of hetero atoms with the help of localized lone pair of electron (LLP) have been evaluated in Table 3.

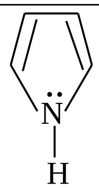
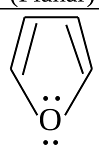
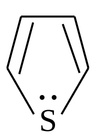
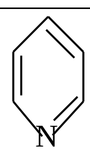
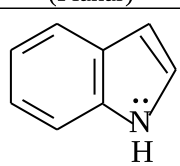
Table 1 T_{SLP} and corresponding hybridization state

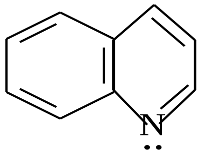
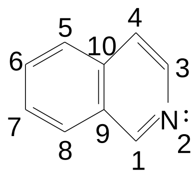
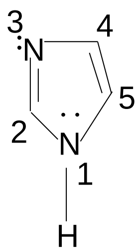
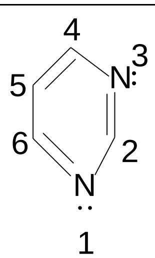
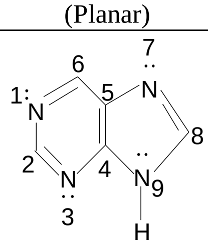
T_{SLP} (Total number of σ bonds + LP)	Nature of Hybridization State	Examples
2	sp	$BeCl_2$, $HgCl_2$,C_2H_2,CO_2,CO,$CdCl_2$, $ZnCl_2$ etc.
3	sp^2	BCl_3, $AlCl_3$,C_2H_4,C_6H_6,SO_2,SO_3,HNO_3, H_2CO_3,$SnCl_2$, $PbCl_2$ etc.
4	sp^3	NH_4^+, BF_4^-, H_2SO_4, $HClO_4$,PCl_3, NCl_3, $AsCl_3$, $HClO_3$,ICl_2^+,OF_2,$HClO_2$,SCl_2,HClO, 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.

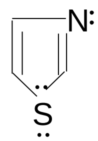
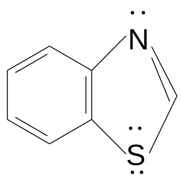
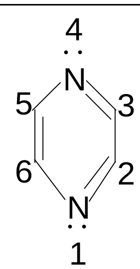
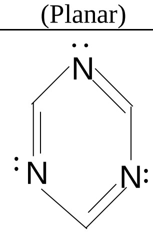
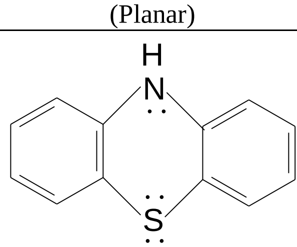
Table 2 Hybridization, Molecular Geometry and Bond Angles without/with lone pair of electrons

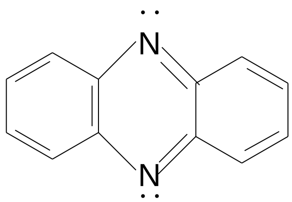
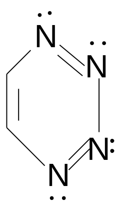
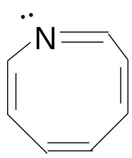
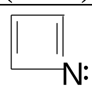
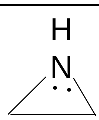
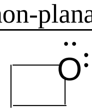
Hybridization	LP	Molecular Geometry (Regular / Normal)	Approximate Bond Angles (Degree)	Examples	LP	Molecular Geometry (Sub-normal)	Approximate Bond Angles (Degree)	Example
sp	0	Linear	180	CO_2, CS_2,$BeCl_2$, $HgCl_2$	-	-	-	-
sp^2	0	Trigonal Planar or Triangular planar	120	BH_3, $AlCl_3$, C_2H_4, BF_3, 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
					02	Bent shape or V-shape	<109.5	H_2O, H_2S, H_2Se
					03	Linear	180	ICl, BrF, ClF
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

Table-3 Hybridization state of Hetero atom in Heterocyclic Compounds with the help of LLP

Heterocyclic Compounds (Planar/non planar)	Number of σ bonds around hetero atom (from single and double bonds) (T_S)	Number of localized Lone Pair of e^-s (LLP)	Total Number of σ bonds around hetero atom (T_{SLLP})	Power on the Hybridization state of the hetero atom **(P_{Hyb}) = (T_{SLLP}) – 1** (Corresponding Hybridization state)
 Pyrrole (Planar)	03	0 (lone pair of electron undergo delocalization,DLP with the ring system)	03	02 (sp^2 N)
 Furan (Planar)	02	01 (out of two lone pair of electrons, one undergo delocalization,DLP and other remain as LLP)	03	02 (sp^2 O)
 Thiophene (Planar)	02	01 (out of two lone pair of electrons of S one undergo delocalization, DLP and other remain as LLP)	03	02 (sp^2 S)
 Pyridine (Planar)	02	01	03	02 (sp^2 N)
 Indole (Planar)	03	0	03	02 (sp^2 N)

 Quinoline (Planar)	02	01	03	02 (sp^2 N)
 Isoquinoline (Planar)	02	01	03	02 (sp^2 N)
 Imidazole (Planar)	03 (N1) 02 (N3)	0 (N1) 01 (N3)	03 03	02 (sp^2 N1) 02 (sp^2 N3)
 Pyrimidine (Planar)	02 (N1) 02 (N3)	01 (N1) 01 (N3)	03 03	02 (sp^2 N1) 02 (sp^2 N3)
 Purine (Planar)	02 (N1) 02 (N3) 02 (N7) 03 (N9)	01 (N1) 01 (N3) 01 (N7) 0 (N9)	03 03 03 03	02 (sp^2 N1) 02 (sp^2 N3) 02 (sp^2 N7) 02 (sp^2 N9)

 Thiazole (Planar)	02 (N) 02 (S)	01 (N) 01 (S) (out of two lone pair of electrons on S, one undergo delocalization,DLP and other remain as LLP)	03 03	02 (sp^2 N) 02 (sp^2 S)
 Benzothiazole (Planar)	02 (N) 02 (S)	01 (N) 01 (S) (out of two lone pair of electrons on S, one undergo delocalization,DLP and other remain as LLP)	03 03	02 (sp^2 N) 02 (sp^2 S)
 Pyrazine (p-diazine) (Planar)	02 (N1) 02 (N1)	01 (N1) 01 (N1)	03 03	02 (sp^2 N1) 02 (sp^2 N4)
 Cyanidine (Planar)	02 (N1,N3 and N5)	01 (N1,N3 and N5)	03	02 (sp^2 N1,N3,N5)
 Phenothiazine (Planar)	03 (N) 02 (S)	0 (N) 01 (S) (out of two LP of S, one undergo delocalization(DLP),	03 03	02 (sp^2 N) 02 (sp^2 S)

		and other remain as LLP)		
 Phenazine (Planar)	02 (both N)	01 (both N)	03	02 (sp^2 both N)
 1,2,3,4-tetrazine (Planar)	02 (N1,N2,N3,N4)	01 (N1,N2,N3,N4)	03	02 (sp^2 All N)
 Azocine (Planar)	02	01	03	02 (sp^2 N)
 Azetine (Planar)	02	01	03	02 (sp^2 N)
 Aziridine (non-planar)	03	01	04	03 (sp^3 N)
 Oxetan (non-planar)	02	02	04	03 (sp^3 O)

Prediction of bond order for diatomic species having (1-20)e$^-$s:

The graphical representation **(Fig. 11)**, 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.

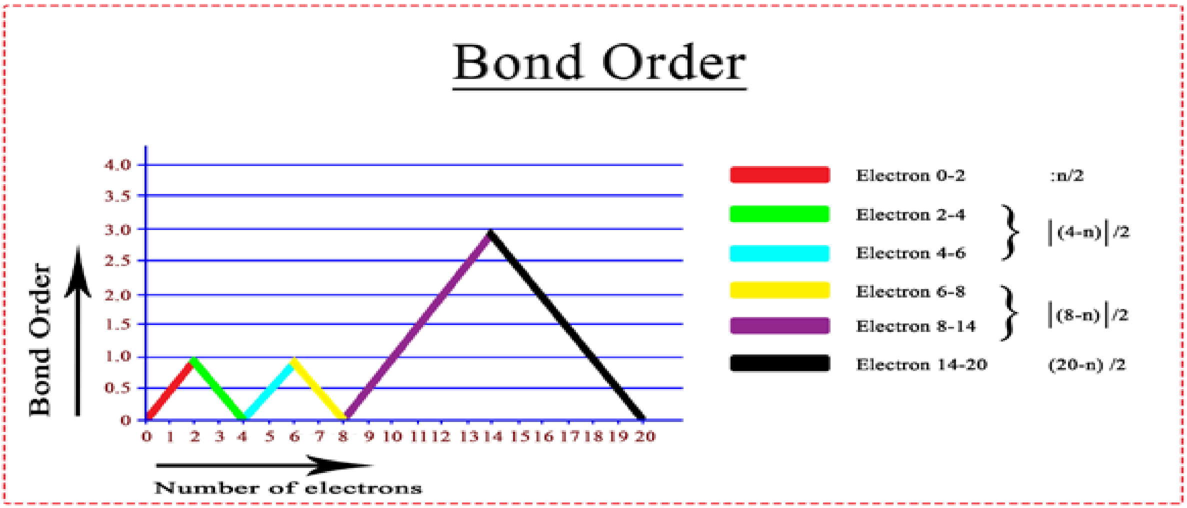


Fig.11 Graphical Representation of B.O. with number of electrons

Prediction of bond order for oxide based acid radicals:

It can be illustrated by the following examples

Eg.

- 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

- AsO_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) = 1

Relation of different parameters (Bond length, Bond Strength, Bond energy, Thermal stability and Reactivity) with Bond order:

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

B.O. α Bond strength;

B.O. α Bond Energy;

B.O. α Bond dissociation Energy;

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

Correlation among / between Literature values of bond-distances (Å) *and* bond dissociation energy (KJ mol^{-1}) *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^- are 1.50, 1.57 and 1.64 (Å) for their predicted bond orders values 1.75, 1.6 and 1.5 respectively ; As-O average bond lengths in AsO_4^{3-} and AsO_3^{3-} are 1.75 and 1.77 (Å) for their predicted bond order values 1.25 and 1.0 respectively which suggests that with increasing Bond-Order bond length decreases.

Literature values of bond dissociation energies of O_2^+, O_2 and O_2^- are respectively 642.9, 493.6 and 395.0 KJ mol^{-1} for their predicted bond orders values 2.5, 2.0 and 1.5 respectively; bond dissociation energies of NO^+, NO and NO^- are respectively 1046.9, 826.9 and 487.8 KJ mol^{-1} for their predicted bond order values 3.0, 2.5 and 2.0 respectively, which suggests that with increasing Bond-Order bond dissociation energy increases.

Magnetic Behavior of Diatomic Species:

Magnetic behavior of diatomic species can be predicted by classify the diatomic species having total number of electrons (1-20) into three different sets and thus calculating the number of unpaired electron/electrons (n) by using three different formulae for three different sets.

Bond order of homo and hetero nuclear diatomic molecules or ions having total number of electrons fall in the range (1-20) can be evaluated from their total number of electrons only without drawing their electronic configuration and their magnetic moments (μ_s) in Bohr Magneton (B.M.) can be evaluated by calculating the number of unpaired electrons have been illustrated in Table 4 and Table 5 respectively.

Table 4 Bond order of diatomic species having (1-20) electrons

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

Table 5 Magnetic moments (μ_s) in B.M. 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

Spin multiplicity and its corresponding spin state:

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

For upward alignment

Eg.

$\boxed{\uparrow}\boxed{}\boxed{}$ $\quad$ $\boxed{\uparrow}\boxed{\uparrow}\boxed{}$ $\quad$ $\boxed{\uparrow}\boxed{\uparrow}\boxed{\uparrow}$

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

$\boxed{\uparrow\downarrow}\boxed{\uparrow}\boxed{\uparrow}$ $\quad$ $\boxed{\uparrow\downarrow}\boxed{\uparrow\downarrow}\boxed{\uparrow}$

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

$\boxed{\uparrow\downarrow}\boxed{\uparrow\downarrow}\boxed{\uparrow\downarrow}$

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

For downward alignment

$\boxed{\downarrow}\boxed{}\boxed{}$ $\quad$ $\boxed{\downarrow}\boxed{\downarrow}\boxed{}$ $\quad$ $\boxed{\downarrow}\boxed{\downarrow}\boxed{\downarrow}$

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

$\boxed{\uparrow\downarrow}\boxed{\downarrow}\boxed{\downarrow}$ $\quad$ $\boxed{\uparrow\downarrow}\boxed{\uparrow\downarrow}\boxed{\downarrow}$

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

For mixed (upward & downward) alignment

$\boxed{\uparrow}\boxed{\downarrow}\boxed{}$

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)

$\boxed{\uparrow}\boxed{\uparrow}\boxed{\downarrow}$

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

For 1, 2, 3, 4, 5, 6 or >6 spin multiplicity values (n+1), where n = number of unpaired electrons, the corresponding spin state will be singlet, doublet, triplet, quartet, quintet and multiplet respectively.

Aromatic and Anti-Aromatic nature of Organic Compounds along with their Omission behavior:

If the compound must be cyclic, planar, conjugated with even and odd number of A value, [where, $A = \pi b + e^{-}p + 1$(constant), here πb = number of π bonds with in the ring system and $e^{-}p$ = delocalized lone pair of electrons (DLP) and each negative charge if present may be treated as one pair of electrons] will be aromatic and anti-aromatic nature respectively.

Stability / reactivity / acidity of different organic compounds with the help of Aromaticity:

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

- Order of stability is aromatic > non aromatic > anti aromatic
- Order of reactivity is Anti-aromatic > non aromatic > aromatic
- Order of Acidity directly proportional to the stability of the Conjugate base

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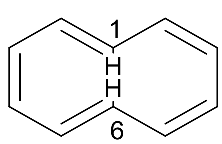
Eg: cyclopentadienyl anion(aromatic) > cyclopentadiene (non-aromatic) > cyclopentadienyl cation (anti aromatic). Hence, cyclopentadiene (its conjugate base i.e. Cyclopentadienyl anion is aromatic in nature) is much more acidic than cycloheptatriene (its conjugate base i.e. Cycloheptatrienyl anion is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

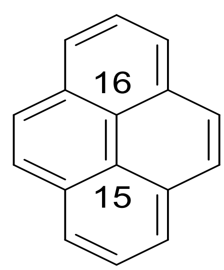
Omission behavior of aromatic and non-aromatic organic compounds:

There are some compounds which do not follow the above rules of A value. Huckel's also cannot explain the aromatic or non-aromatic behavior of these compounds. These compounds have been represented below.

Cyclodecapentaene (Fig. 12), is non aromatic due to the interaction of the hydrogen of 1 and 6, it is non planar, although here, A = πb + DLP + 1(constant) = 5 + 0 + 1 = 6 (even number). Pyrene **(Fig. 12)**, is a polycyclic aromatic hydrocarbon consisting of four fused benzene rings, resulting in a flat aromatic system. It has 8 π bonds and zero (0) DLP. Here, A = 8 + 0 + 1 = 9 (odd number). But still it is aromatic instead of anti-aromatic because double bonded C_{15}-C_{16} does not take part in resonance.



Cyclodecapentaene



Pyrene

Fig. 12 Geometry of Cyclodecapentaene and Pyrene

Aromatic and Anti-Aromatic behavior of Heterocyclic Compounds along with their omission nature:

The heterocyclic compound having cyclic, planar, conjugated (i.e. all the carbon atoms having same state of hybridization, sp^2) with even number of 'A' value will be treated as aromatic in nature and with odd number of 'A' value will be treated as anti-aromatic in nature.

In case of a multi hetero atom based heterocyclic compound, containing both DLP and LLP hetero atoms, Aromatic and Anti Aromatic behavior should be predicted with respect to DLP based hetero atom only.

Eg. Benzothiazole (Fig. 13), is a multi hetero atom based heterocyclic compound, containing both DLP and LLP hetero atoms. Here, for N, DLP = 0 , LLP = 1 and for S, DLP = 1, LLP =1, so, in this case 'A' value should be calculated with respect to S only not N. Here, A = 4 + 1 + 1 = 6 (even no) = Aromatic.

But when heterocyclic compounds contain both LLP based hetero atoms then Aromaticity should be predicted with respect to that hetero atom which contains lowest possible position number as per IUPAC nomenclature or any one of the hetero atom.

Eg. Imidazole (Fig. 13) is a multi hetero atom based hetero cyclic compound in which, N1 is DLP based hetero atom and N3 is LLP based hetero atom. In this case Aromaticity should be predicted with respect to the DLP based hetero atom N1. For N1, A = πb+DLP+1(constant) = 2+1+1 = 4 (even No) - Aromatic

Eg. Pyrimidine (Fig. 13) is a multi hetero atom based hetero cyclic compound in which, both N1 & N3 are in same environment based hetero atoms (LLP based hetero atoms). In this case Aromaticity should be predicted with respect to N1 (lowest possible position number as per IUPAC nomenclature). For N1, A = πb+DLP+1(constant) = 3+0+1 = 4 (even no) – Aromatic.

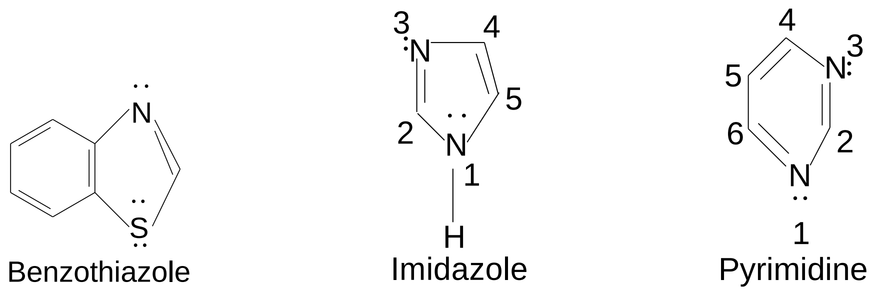


Fig. 13 Structure of Benzothiazole, Imidazole and Pyrimidine

Omission behavior of some heterocyclic compounds with respect to their Aromatic / Anti Aromatic and Non Aromatic nature

Heterocyclic compounds containing different DLP based hetero atoms (one *contains vacant d orbitals*)*:*

In Phenothiazine (Fig. 14), there is two DLP based hetero atoms N and S. In between N and S, since S having vacant d orbitals, so, in this case 'A' value will be predicted with respect to DLP based S hetero atom which contains vacant d orbitals only. Here, A = πb + DLP + 1(constant) = 6 +1+1 = 8 (even no) = Aromatic.

Heterocyclic compounds containing same DLP based heteroatom having no d orbitals:

Omission behavior of some heterocyclic compounds will be observed (Fig. 14), when there, is at least two hetero atoms (same or different) but both the hetero atoms do not have any d orbitals (such as O,N etc.) and they are in DLP based environment in the ring system.

These molecules have been studied with advanced molecular orbital techniques known as 'ab initio calculations'. *'Ab initio quantum chemistry methods'* are computational chemistry methods based on quantum chemistry [28].

In the case of 1,2-dioxin, 1,4-dioxin and dibenzo-1,4-dioxin there is DLP based O atoms in all the molecules but still they will be non-aromatic due to prevention of significant free electron delocalization (makes non conjugated). The π electrons from the carbon bonds and the lone pair electrons on the oxygen atoms do not overlap to a significant degree due to absence of vacant d orbitals in both O atoms in each case (pπ-dπ overlap is not possible here in conjugation). It makes these molecules non conjugated and thus allows the molecules to become non aromatic instead of aromatic (A value = even No).

In the heterocyclic compounds, where, there is two DLP based N atoms instead of two DLP based O atoms or there is one DLP N atom along with one DLP O atom, the same phenomena of non-aromatic behavior will be observed. Because, both N and O atoms do not have any vacant d orbitals, and hence pπ-dπ overlap is not possible here in conjugation.

Heterocyclic compounds containing same DLP based hetero atoms having vacant d orbitals:

1,4-dithiin and 1,2-dithiin heterocyclic compounds (Fig. 14) are anti-aromatic, here both S atoms, having vacant d orbitals, contain one DLP and one LLP and here both DLP of both S atoms participate in the delocalization. Hence, for the prediction of 'A' value, consider both DLP (DLP = 2). Here, A = πb + DLP + 1 (Constant) = 2 + 2 + 1 = 5 (odd No) = Anti Aromatic.

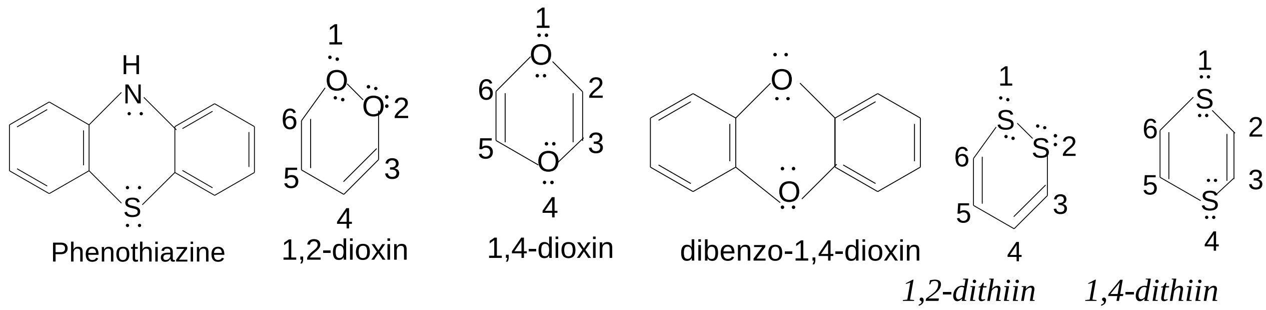


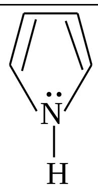
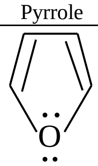
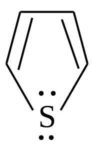
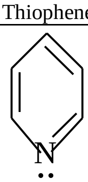
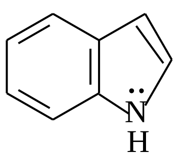
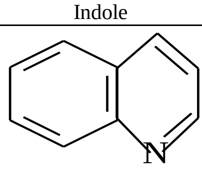
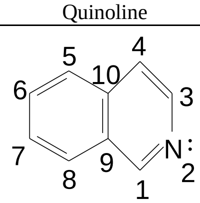
Fig.14 Structure of phenothiazine, 1,2-dioxin, 1,4-dioxin, dibenzo-1.4-dioxin and 1,2-dithiin and 1,4-dithiin

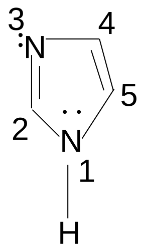
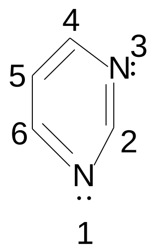
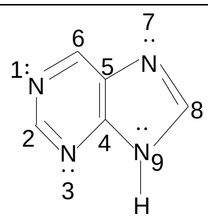
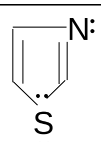
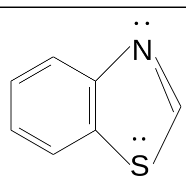
Aromatic, anti-aromatic and non-aromatic behavior of organic compounds including heterocyclic compounds have been illustrated with adequate number of examples in Table 6 and 7 respectively.

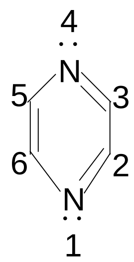
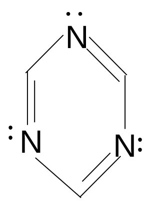
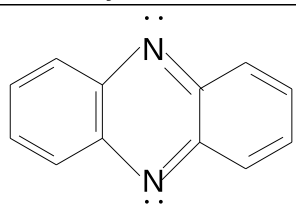
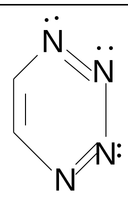
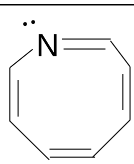
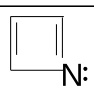
Table 6 Aromatic, anti-aromatic and non-aromatic behavior of organic compounds

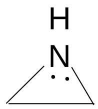
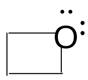
Organic Compound (Cyclic, Planar/Cyclic, non-planar)	*πb value [πb =number of π bonds with in the ring system]*	*e^-p value [e^-p = number of delocalized electron pair outside or adjacent to the ring system]*	*A value [A = πb + e^-p + 1(constant)] (even no/odd no)*	*Nature of compound (aromatic/anti-aromatic/non 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 sp^3 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 sp^3 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 sp^3 hybridized carbon atom adjacent to positive charge)	3 π bonds	0	3 + 0 + 1 = 4 (even no)	Non aromatic

Table 7 Aromatic-Anti Aromatic and Non Aromatic behavior of heterocyclic compounds with DLP

Hetero Cyclic Compound (Cyclic, Planar, Conjugated)	πb value [πb =number of π bonds with in the ring system]	DLP	A value [A = πb + DLP + 1(constant)] (even No /odd No)	Remark on Nature of compound (Aromatic/Anti Aromatic)
 Pyrrole	2	1	2 + 1 + 1 = 4 (even No)	Aromatic
 Furan	2	1 (Here out of two lone pairs on O only one LP take part in delocalization)	2 + 1 + 1 = 4 (even No)	Aromatic
 Thiophene	2	1 (Here out of two lone pairs on O only one LP take part in delocalization)	2 + 1 + 1 = 4 (even No)	Aromatic
 Pyridine	3	0	3 + 0 + 1 = 4 (even No)	Aromatic
 Indole	4	1	4 + 1 + 1 = 6 (even No)	Aromatic
 Quinoline	5	0	5 + 0 + 1 = 6 (even No)	Aromatic
 Isoquinoline	05	0	5 + 0 + 1 = 6 (even No)	Aromatic

 Imidazole	02	01 (N1)	2 + 1 + 1 = 4 (even No)	Aromatic
 Pyrimidine (m-diazine)	03	0 (N1)	3 + 0 + 1 = 4 (even No)	Aromatic
 Purine	04	01 (N9)	4 + 1 + 1 = 6 (even No)	Aromatic
 Thiazole	02	01 (S)	2 + 1 + 1 = 4 (even No)	Aromatic
 Benzothiazole	04	01 (S)	4 + 1 + 1 = 6 (even No)	Aromatic

 Pyrazine (p-diazine)	03	0	3 + 0 + 1 = 4 (even No)	Aromatic
 Cyanidine	03	0	3 + 0 + 1 = 4 (even No)	Aromatic
 Phenazine	07	0	7 + 0 + 1 = 8 (even No)	Aromatic
 1,2,3,4-tetrazine	03	0	3 + 0 + 1 = 4 (even No)	Aromatic
 Azocine	04	0	4 + 0 + 1 = 5 (odd No)	Anti aromatic
 Azetine	02	0	2 + 0 + 1 = 3 (odd No)	Anti aromatic
Hetero Cyclic Compound (Cyclic, non-planar)	πb value [πb =number of π bonds with in the ring system]	DLP	A value [A = πb + DLP + 1(constant)] (even No/odd No)	Remark on Nature of compound

 Aziridine	-	-	-	Non Aromatic (non planar – sp^3)
 Oxetan	-	-	-	Non Aromatic (non planar – sp^3)

Calculation of chemical bonds in Straight Chain and Cycloalkene System:

Chemical bonds (π-bonds, σ-bonds, single and double bonds) in the open chain and cyclic olefinic hydrocarbons having complex molecular formulae like $C_{176}H_{250}$, $C_{2000}H_{2000}$ can be calculated without drawing their structures by using different formulae, involving the number of carbon and hydrogen atoms only.

Calculation of chemical bonds (π bonds, σ bonds, single and double bonds) in open chain and cyclic olefinic hydrocarbons without drawing their structures have been illustrated in Table 8 and Table 9 respectively.

Table 8 Calculation of bonds in open chain olefinic hydrocarbons

Example (C_xH_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_2H_4	$H_2C=CH_2$	1	5	4	1
C_3H_6	$H_2C=CH-CH_3$	1	8	7	1
C_3H_4	$H_2C=C=CH_2$	2	6	4	2
C_4H_8	i)$H_2C=CH-CH_2-CH_3$ ii)$H_3C-HC=CH-CH_3$	1	11	10	1
C_4H_6	i)$H_2C=C=CH-CH_3$ ii)$H_2C=CH-CH=CH_2$	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
$C_{99}H_4$	-	98	102	4	98

Table 9 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

Calculation of chemical bonds in Straight Chain and Cycloalkyne System:

Chemical bonds (π-bonds, σ-bonds, single and triple bonds) in the open chain alkynes and cycloalkynes can be calculated in the same way by using different formulae, involving the number of carbon and hydrogen atoms without drawing their structure as follows.

E.g.: In cycloheptyne (C_7H_{10}), X =7, Y = 10, therefore, number of π bonds (P_c) = (2x7-10)/2 = 2; number of σ bonds (S_c) = (7+10) = 17; numbers of single bonds (A_c) = [{(2X+5Y)/2}]/2 = [{(2x7+5x10)/2}]/2=32/2 = 16 and number of triple bonds (T_c) = [{(2X-Y)/2}]/2 = [{(2 x 7 – 10)/2}]/2 = 2/2 = 1.

Calculation of chemical bonds (π bonds, σ bonds, single and triple bonds) in open chain alkynes without drawing their structures have been illustrated in Table 10.

Table 10 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

CONCLUSION

It may be expected that these time economic innovative mnemonics would go a long way to help 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 to use these time economic innovative mnemonics in the field of chemical education.

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