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Innovative Mnemonics in Chemical Education - A Review Article

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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 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.

1. Introduction

The conventional methods [1-13] 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. Keeping this in mind, in this survey, I have introduced some innovative methods [14]-[23] to make chemistry metabolic, time economic and interesting. Here, I have tried to discuss them abruptly.

2. Methods

2.1. 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 differ 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 (1931), first proposed the Hybridization in order to explain the structure of molecules such as methane (CH_4) using atomic orbitals.

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. Innovative Time Economic Mnemonics for the Prediction of Hybridization State *sp, sp², sp³*

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

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

Power on the Hybridization state of the central atom =
(Total no of σ bonds around each central atom -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 σ bond, in 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.

2.1.2. Innovative Time Economic Mnemonics for the 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:-

a. 5σ bonds = 4σ bonds + 1 additional σ bond = sp3d hybridization
b. 6σ bonds = 4σ bonds + 2 additional σ bonds = sp3d2 hybridization
c. 7σ bonds = 4σ bonds + 3 additional σ bonds = sp3d3 hybridization

2.1.3. Predicting the Hybridization of Heterocyclic Compounds

In this case, state of s-p hybridization of hetero atoms 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:

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

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

DLP = Delocalized lone pair electrons through resonance (Number of LP e⁻s on the hetero atom, which is directly attached with single bonds only).

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

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. 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.

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

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.

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 which have been presented in Table 7 and thus magnetic moment (μ_s in B.M.) can be evaluated in the following way:
Determination of Number of Unpaired Electrons

2.4.1. F-1 (For Set-1) – For 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 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 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. 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.

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. Identifying Aromatic and Anti-Aromatic Compounds

It was first devised by Huckel in 1931. 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).

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. 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. 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.

2.7.1. 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.

2.7.2. 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.

2.8. 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.

2.8.1. 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.

2.8.2. 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 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 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 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 $T_c = [\{(2X-Y)/2\}]/2$;

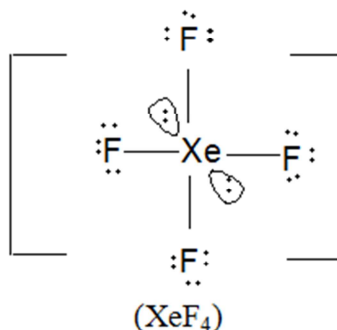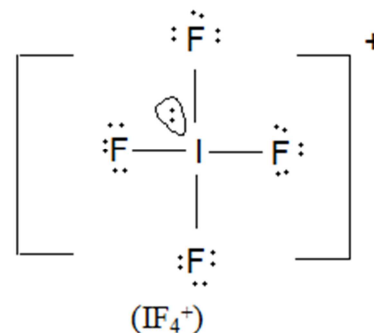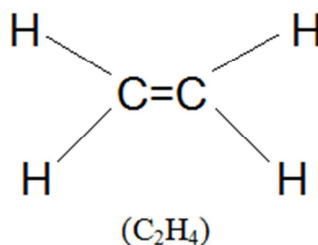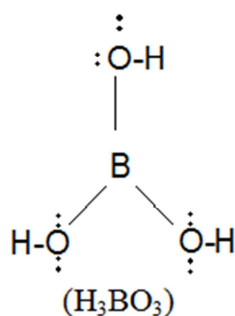where, X = number of carbon atoms;
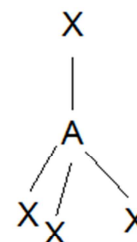Y = number of hydrogen atoms

3. Tables and Figures

Figure 1. *Geometry of H_3BO_3, C_2H_4, IF_4^+, XeF_4.*
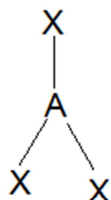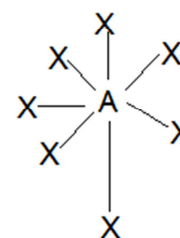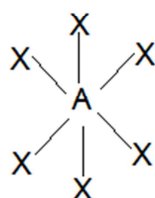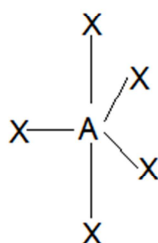
Figure 2. *Regular / Normal Molecular Geometry without Lone pair of electrons.*

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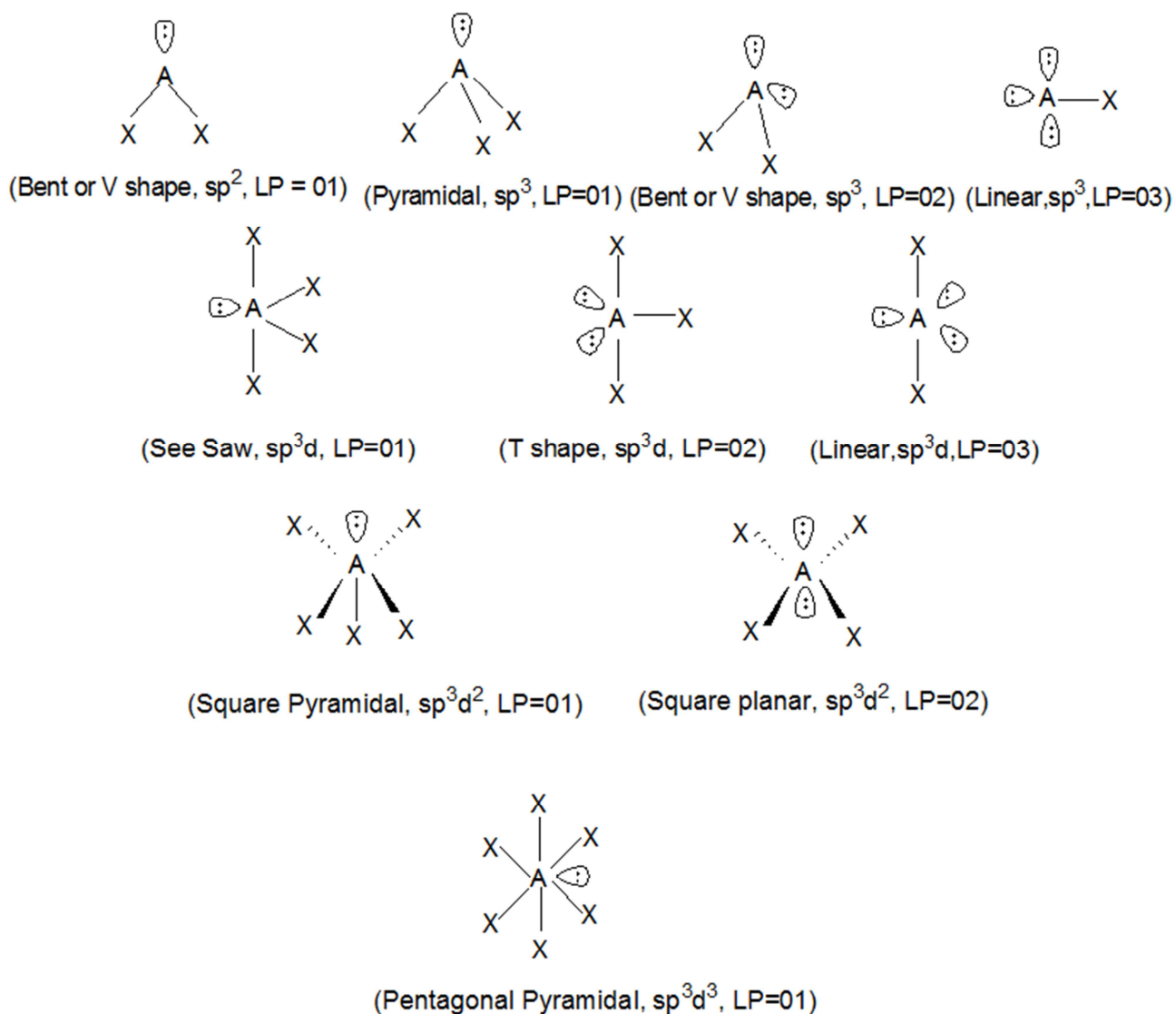
(Pentagonal Pyramidal, sp^3d^3, LP=01)

Figure 3. *Sub-normal Molecular Geometry with Lone pair of electrons.*

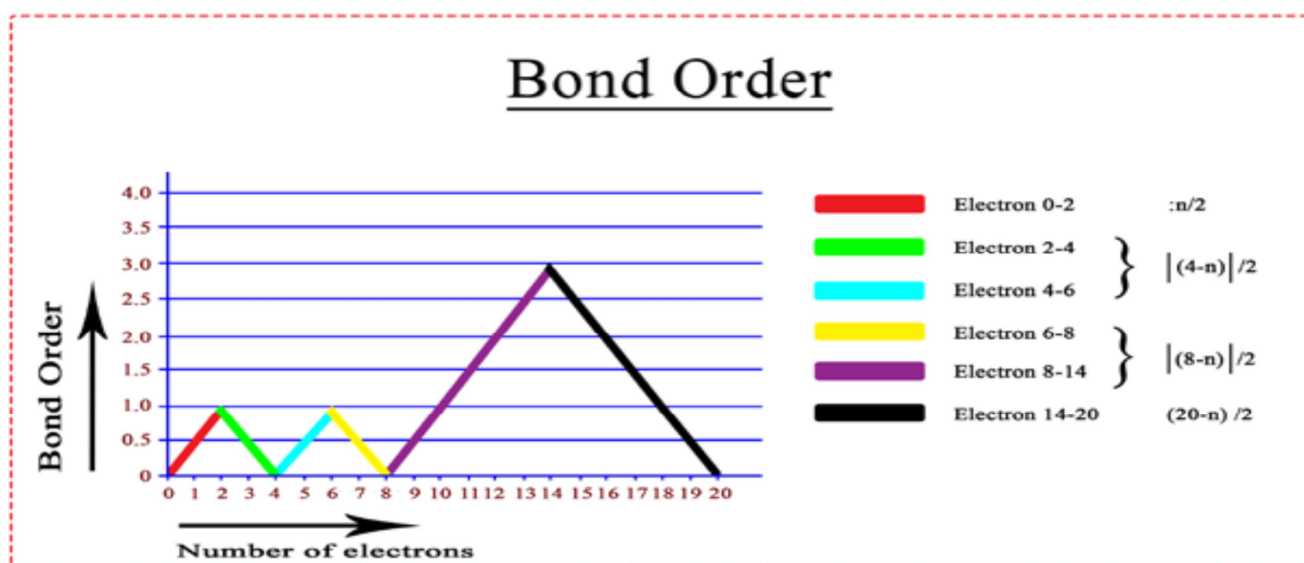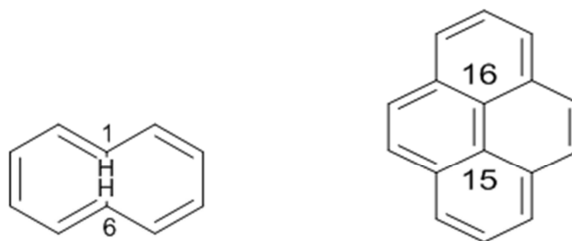**Figure 4.** *Graphical Representation of B.O. with number of electrons.*

Figure 5. Geometry of Cyclodecapentaene and Pyrene.

Table 1. Number of σ bonds and its 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.

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, 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
					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 atoms in some Heterocyclic Compounds.

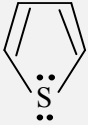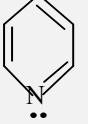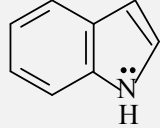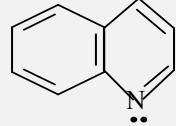| Heterocyclic Compounds	TNBS (Total number of bonds around hetero atom excluding H Bond)	DLP (Delocalized Lone Pair of e⁻s)	Total Power (X) = TNBS + DLP	Hybridization State
Pyrrole	2	1	3	sp^2
Furan	2	1 (01 LLP & 01 DLP)	3	sp^2

Heterocyclic Compounds	TNBS (Total number of bonds around hetero atom excluding H Bond)	DLP (Delocalized Lone Pair of e⁻s)	Total Power (X) = TNBS + DLP	Hybridization State
Thiophene	2	1 (01 LLP & 01 DLP)	3	sp^2
Pyridine	3	0 (01 LLP)	3	sp^2
Indole	2	1	3	sp^2
Quinoline	3	0 (01 LLP)	3	sp^2

Table 4. Bond order 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

Table 5. 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

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
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

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 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 (Here 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

Table 7. *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 8. *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

Table 9. *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

4. 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. 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 = sp^3.

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, altogether 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) (Figure 1), 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, 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 (Figure 1). So, in this case, power of the hybridization state of both C = 3-1 = 2 i.e. hybridization state of both C's are sp^2.

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

Eg:

a. IF_4^+: I has 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 (Figure 1). So, altogether there are 5 σ bonds. So, 5σ bonds = 4 σ bonds + 1 additional σ bond = sp^3d hybridization

b. XeF_4: In the Lewis structure of XeF_4 (Figure 1), Xe, an inert gas, consider 8 e⁻s in its outermost shell, 04 of which form 04 Xe-F sigma bonds and there is 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 incase of anionic species, added requisite electron with the outermost electrons of the central atom. Examples have been explored in Table 1.

Geometry of simple molecules or ions:

In absence of lone pair of electrons a molecule or ion exhibit regular geometry (Figure 2, Table 2). For sp, sp^2, sp^3, sp^3d, sp^3d^2 and sp^3d^3 hybridization state, regular geometry will be linear, trigonal planar, tetrahedral, trigonal bipyramid, octahedral and pentagonal bipyramid respectively, where as for the same hybridization state in presence of lone pair of electrons they exhibit sub normal geometry (Figure 3, Table 2).

Prediction of hybridization state of hetero atom in the heterocyclic compounds:

Prediction of hybridization state of hetero atom in the heterocyclic compounds with the help of delocalized lone Pair of electrons (DLP) have been illustrated in Table 3.

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

The graphical representation (Figure 4), 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. Bond order prediction with examples have been represented in Table 4.

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. Examples are

given in Table 5.

*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:

↑

↑   ↑

↑   ↑   ↑
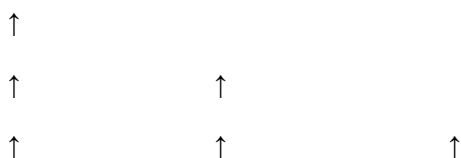
Spin multiplicity = (n +1) = (1+1) = 2 (spin state = doublet); (2+1) = 3 (spin state = triplet) and (3 + 1) = 4 (spin state = quartet) respectively.
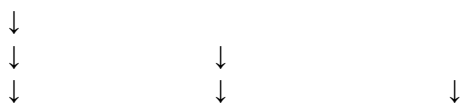
↑↓   ↑   ↑
↑↓   ↑↓   ↑
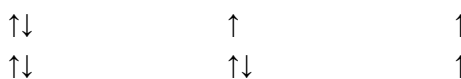
Spin multiplicity = (n +1) = (2 + 1) = 3 (in this case ignore paired electrons) (spin state = triplet) and (1 + 1) = 2 (spin state = doublet)

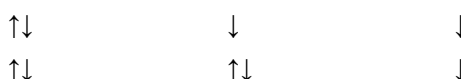↑↓   ↑↓   ↑↓

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

For downward alignment

↓

↓   ↓

↓   ↓   ↓

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.

For mixed (upward & downward) alignment

↑   ↓

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 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 behavior of Organic Compounds:

If the compound must be cyclic, planar, conjugated with even and 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 = 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. Examples of aromatic, anti aromatic and non aromatic organic compounds can be shown in Table 6.

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

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 (Figure 5), 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 (Figure 5), 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.

Calculation of chemical bonds (π-bonds, σ-bonds, single and double bonds) in Straight Chain and

Cycloalkene System:

Chemical bonds in the straight chain olefin and cycloalkene systems can be calculated by using different formulae, involving the number of carbon atoms and number of hydrogen atoms (Table 7 & Table 8).

Calculation of chemical bonds (π-bonds, σ-bonds, single and triple bonds) in Straight Chain and Cycloalkyne System:

Chemical bonds in the straight chain alkyne can be calculated by using different formulae, involving the number of carbon atoms and number of hydrogen atoms (Table 9) and that of cycloalkene system can be calculated in the same way by using different formulae, involving the number of carbon hydrogen atoms 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.

5. Conclusion

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

Acknowledgements

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