Dr. Arijit Das

Proposed 22 Innovative Teaching Methodologies of Chemistry

Innovative Methodology 1:

New Innovative Methods for Prediction of Hybridization State in a Very Short Time

Publication Year: 2011

Innovative Methodologies 2 & 3:

New Innovative Methods for Determination of Spin Multiplicity, Spin State and Magnetic Properties of Diatomic Hetero Nuclear Molecules or Ions in a Very Short Interval of Time

Publication Year: 2011

Innovative Methodologies 4 & 5:

New Methods for Prediction of Bond Order of Mono and Diatomic Homo and Hetero Nuclear Molecules or Ions Having (1-20)E S and Oxide Based Acid Radicals Without Mot – a Rapid Innovative Approach

Publication Year: 2011

Innovative Methodologies 6 & 7:

New Innovative Methods for IUPAC Nomenclature of Bicyclo and Spiro Compounds in Organic Chemistry

Publication Year: 2013

Innovative Methodology 8 :

Rapid calculation of the number of π-bonds, σ-bonds, single and double bonds in aliphatic unsaturated open chain and cyclic olefinic hydrocarbons

Publication Year: 2014

Innovative Methodology 9:

Rapid calculation of the number of π-bonds, σ-bonds, single and triple bonds in aliphatic unsaturated open chain and cycloalkynes

Publication Year: 2014

Innovative Methodology 10:

Time Economic Innovative Methodology on the Prediction of Hybridization State of Heterocyclic Compounds

Publication Year: 2014

Innovative Methodologies 11 & 12:

A Rapid and Innovative Method for the Identification of Aromatic and Anti-Aromatic Nature of Organic Compounds

Publication Year: 2013

Innovative Methodologies 13 & 14:

Bond-Order and Magnetic Behavior of Diatomic Species without Molecular Orbital Theory

Publication Year: 2017

Innovative Methodologies 15 & 16:

Lone Pair Electron Discriminate Hybridization with Aromatic and Anti Aromatic Behavior of Heterocyclic Compounds – Innovative Mnemonics

Publication Year: 2018

Innovative Methodologies 17, 18 & 19:

Predicting the Hybridization State: A Comparative Study between Conventional and Innovative Formulae

Publication Year: 2020

Innovative Methodology 20:

IUPAC Nomenclature of Higher Alkanes — Innovative Mnemonics

Publication Year: 2021

Innovative Methodologies 21 & 22:

Classification of Negative Charge Discriminate Hybridization with Aromatic and Anti-Aromatic Behavior of Organic Compounds – Innovative Mnemonics

Publication Year: 2021

Invented 40 Formulae

Determination of hybridization state like sp, sp^2, sp^3 for simple molecules or ions followed the following formula

Formula 1 (2011):

Power of the Hybridization state of the centre atom = (Total no of σ bonds around each centre atom -1)

All single (-) bonds are σ bond, in double bond (=) there is one σ and 1π, in triple bond there is one σ and 2π. In addition to these each lone pair (i.e.no of electrons in the outermost orbit which should not take part in bond formation) and Co-ordinate bond can be treated as one σ bond.

Prediction of Aromatic behavior:

Formula 2 (2013):

$A = \pi b + e^{-}p + 1$(constant) = even no (Aromatic)

Here, πb = number of π bonds within the ring system and $e^{-}p$ = number of electron pair outside or adjacent to the ring system i.e. ring contains hetero atom (atom contains lone pair of electrons) which can undergo delocalization and each negative charge if present may be treated as one pair of electrons.

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

Prediction of Anti-aromatic behavior:

Formula 3 (2013):

In this 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.

$A = \pi b + e^{-}p + 1$(constant) = odd no (Anti Aromatic)

IUPAC Nomenclature of Bicyclo Compounds:

The format of IUPAC nomenclature for non-substituted bicyclo compounds is

Formula 4 (2013):

'bicyclo[a,b,c]alkane'

where, 'a' and 'b' are the maximum and minimum number of points respectively in the fused ring system excluding common points and variable 'c' = no of common points (cp) – 2.

IUPAC Nomenclature of Spiro Compounds:

Formula 5 (2013):

'spiro[a,b]alkane'

where, 'a' and 'b' are the minimum and the maximum number of points respectively in the fused ring system excluding common point (cp).

The format of IUPAC nomenclature for mono substituted bicyclo and *spiro* compounds are

Formula 6 (2013):

'x-substituent bicyclo[a,b,c]alkane'

or

'x-substituent spiro[a,b,c]alkane'

Prediction of Hybridization state of Hetero atom in Heterocyclic Compounds:

Formula 7 (2014):

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

Prediction of Bond order without Molecular Orbital Theory:

Formula 8 (2014):

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

Bond order = n/2

Formula 9 (2014):

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

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

Formula 10 (2014):

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

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

Formula 11 *(2014):*

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, '| |' indicates Mod function i.e. the value of bond order is always positive]

Prediction of Bond-Order of oxide based acid radicals:

Formula 12 *(2014):*

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)

Prediction Magnetic Behavior of Diatomic Species:

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:

Formula 13 *(2014):*

(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 = [| (NED - total e^-s) |]

Here, NED = next digit i.e. digit next to minimum digit and '| |' indicates mod function. Eg:Molecules or ions having (1-3)e^-s, in this case NED = 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.

Formula 14 (2014):

(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 = [| (PED - total e^-s) |]

Here, PED = Penultimate electron digit (i.e. before last electron).

For the molecules or ions containing (10-13) and (16-19)e^-s the PED value will be 12 and 18 respectively. Hence, the value of n = [| (12 - total e^-s) |] and [| (18 - total e^-s) |] respectively.

Formula 15 (2014):

(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)]

Evaluating Spin Multiplicity:

Formula 16 (2014):

Species having unpaired electrons in upward alignment (↑):

In this case, **spin multiplicity = (n+1)**

where n = number of unpaired electrons

Formula 17 (2014):

Species having unpaired electrons in downward alignment (↓):

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

Here (-ve) sign indicate downward arrow

Formula 18 (2014):

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.

Calculating of π-bonds, σ-bonds, single and double bonds in Straight Chain and Cycloalkene Systems:

For Open Chain Aliphatic Hydrocarbons:

(i) **Calculation of π-bonds and double bonds (P):**

The number of π bonds (P) or double bonds for a straight chain olefin is

***Formula 19** (2014):*

$$P= [(2X-Y)/2] + 1$$

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):**

***Formula 20** (2014):*

$$S = [X + Y - 1]$$

(iii) Calculation of Single bonds (A):

***Formula 21** (2014):*

$$A = [(3Y/2)-2]$$

where A = number of single bonds and Y is number of hydrogen atoms.

For Cyclic aliphatic olefinic hydrocarbons:

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

The number of π bonds or double bonds (P_c) for an aliphatic cyclic olefin is

***Formula 22** (2014):*

$$P_c= [(2X-Y)/2]$$

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

(ii)Calculation of σ-bonds (S_c):

***Formula 23** (2014):*

$$S_c = [X + Y]$$

iii) Calculation of Single bonds (A_c):

Formula 24 (2014):

$$A_c = [3Y/2]$$

Calculating of π-bonds, σ-bonds, single and triple bonds in Straight Chain Alkyne and Cycloalkyne Systems:

Open Chain Aliphatic Alkynes:

(i) **Calculation of π-bonds (P):**

Formula 25 (2014):

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

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

ii) Calculation of σ-bonds (S):

Formula 26 (2014):

$$S = [X+Y-1]$$

iii) Calculation of Single bonds (A):

Formula 27 (2014):

$$A = [\{(2X+5Y)/2\} - 3]/2$$

(iv) Calculation of Triple bonds (T):

Formula 28 (2014):

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

Cycloalkynes:

(i) **Calculation of π-bonds (P_c):**

Formula 29 (2014):

$$P_c = [(2X-Y)/2]$$

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

(ii) Calculation of σ-bonds (S_c):

Formula 30 (2014):

$$S_c = [X + Y]$$

(iii) Calculation of Single bonds (A_c):

Formula 31 (2014):

$$A_c = [\{(2X+5Y)/2\}]/2$$

X = number of carbon atoms and Y = number of hydrogen atoms.

(iv) Calculation of Triple bonds (T):

Formula 32 (2014):

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

Prediction of sp, sp^2, sp^3 Hybridization state of simple molecules or ions :

Formula 33 (2018):

Prediction of sp, sp^2, and sp^3 hybridization state for simple molecules or ions

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 [26, 29, 31].

Prediction of sp^3d, sp^3d^2, sp^3d^3 Hybridization state of simple molecules or ions :

Formula 34 (2018):

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

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

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

Predicting hybridization state of hetero atom in different heterocyclic compounds:

Formula 35 (2018):

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.

Prediction of Aromatic, Anti Aromatic behavior of Heterocyclic Organic Compounds with DLP:

Formula 36 (2018):

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

Formula 37 (2018):

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.

Predicting hybridization state (sp, sp^2, sp^3) of carbon atom bearing positive or negative charge in different non heterocyclic organic compounds:

Formula 38 (2021):

Power on the hybridization state of the central atom or ions (P_{Hyb}) = (T_{SLNC}) – 1

where, P_{Hyb} = power on the hybridization state of the carbon atom bearing negative charge, T_{SLNC} = (Total no of σ bonds around each carbon atom + LNC), LNC = localized negative charge. During prediction of the hybridization state of carbon bearing positive charge ignore the positive charge.

Formula 39 (2021):

Evaluation of 'A' Value to predict Aromatic and Anti Aromatic Nature

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

Formula 40 (2021):

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

where, πb = number of π bonds within the ring system, DNC = delocalized negative charge on carbon atoms of ring system.

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Federation of African Societies of Chemistry, Ethiopia, Africa

Link: https://www.ajol.info/index.php/ajce/article/view/176086

Dr. Arijit Das

Proposed Six (06) Advanced Laboratory Experiments

PC Experiment-1: Separation of Group II Metal ions (Pb^{2+} & Cu^{2+}) by 10% KI Solution

Publication Year: 2023

PC Experiment-2: Separation of Group IV Metal ions (Ni^{2+} & Co^{2+}) by 5% NH_4OH solution

Publication Year: 2023

PC Experiment-3: Separation of Group II and Group III Metal ions (Cu^{2+} & Fe^{3+}) by 1(N) $K_4[Fe(CN)_6]$ solution

Publication Year: 2023

PC Experiment-4: Separation of Group II and Group IV Metal ions (Cu^{2+} & Co^{2+}) by 10% NH_4OH solution

Publication Year: 2023

PC Experiment-5: Separation of Group III Metal ions (Fe^{3+} & Cr^{3+}) by 1(N) $K_4[Fe(CN)_6]$ solution

Publication Year: 2024

PC Experiment-6: Separation of Group III Metal ions (Mo^{6+} & W^{6+}) by 1(N) $CuCl_2$ solution

Publication Year: 2024

ADVANCED LAB EXPERIMENTS INDEXED GLOBALLY BY THE

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Federation of African Societies of Chemistry, Ethiopia, Africa

Link: https://www.ajol.info/index.php/ajce/article/view/276634

Launched Two Educational Tools in US

Free Educational AI Tool-1:

‘Hydrocarbons Parser’

Published by minerazzi.com, US

Publication Year: 2015

Link: https://arijitchemistryworld.in/tool-software/

Link: http://www.minerazzi.com/tools/hydrocarbons/parser.php

Free Educational AI Tool 2:

‘Bond Order Calculator‘

Published by minerazzi.com, US

Publication Year: 2018

Link: https://arijitchemistryworld.in/tool-software/

Link: http://www.minerazzi.com/tools/bond-order/calculator.php

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INNOVATIVE BOOK PUBLISHED ENTITLED

‘Innovative Mnemonics in Chemical Education: A Handbook for Classroom Lectures’

DATED: 11Sept 2019 (Online) & 1st Nov-2019 (Hard Back)

Publisher**: Cambridge Scholars Publishing, Lady Stephenson Library, Newcastle upon Tyne,NE6 2PA, UK,** **Link**: https://www.cambridgescholars.com/innovative-mnemonics-in-chemical-education.

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