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Lone Pair of Electrons Discriminate Hybridization with Aromaticity in the Heterocyclic Compounds - Innovative Mnemonics

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Abstract In this approach, formulae based mnemonics by counting lone pair of electrons (localized or delocalized) have been highlighted by innovative and time economic way to enhance interest of students' who belong to paranoia zone of chemistry for the prediction of aromatic behavior and hybridization state of heterocyclic compounds. In order to ameliorate the field of chemical education, I have taken an enterprise to hub two economic mnemonics including two different formulae. This article encourages students to solve multiple choice type questions (MCQs) at different competitive examinations for a time being in an economic ground for the prediction of aromaticity and hybridization state of heterocyclic compounds containing two or more hetero-atoms. Educators can use these mnemonics in their teaching style in the classroom lectures after discussing conventional methods to make chemistry intriguing because the use of mnemonics in classroom lectures is an essential tool to become a distinguished educator.

Keywords: *high school, under graduate student, graduate student, post graduate student, chemical education research, heterocyclic compound, DLP, LLP, aromaticity and hybridization*

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1. Introduction

The conventional methods [1-7] for determination of hybridization state and aromatic nature of heterocyclic compound is time consuming. Keeping this in mind, in this article, I have introduced two innovative mnemonics, economically sound by using two formulae to make heterocyclic chemistry metabolic and inspiring for students.

Time Economic Innovative Mnemonics in Heterocyclic Chemistry

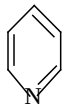
Classification of Lone Pair of Electrons

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 delocalized lone pair of electron (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.

Hybridization state theory

Pauling (1931) first developed the Hybridization state theory in order to explain the structure of molecules such as methane (CH_4). Pauling's 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 to excuse the structures of organic and inorganic compounds along with their related problems.

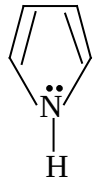
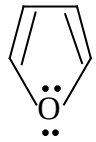
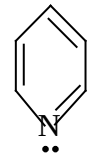
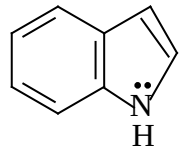
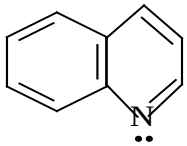
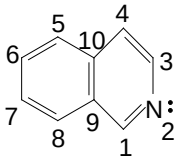
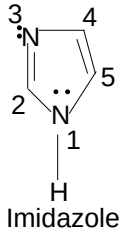
Innovative Mnemonics on the Prediction of Hybridization state in Heterocyclic Compounds with LLP

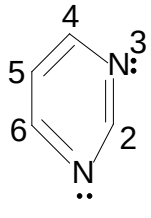
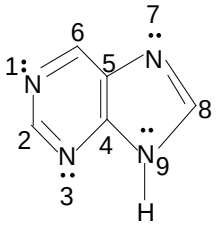
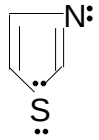
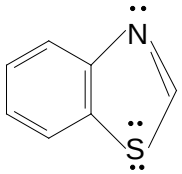
Formula used for the determination of hybridization state:

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

All single (-) bonds are σ bond, in double bond (=) there is one σ and 1π. In addition to these each localized lone pair of electron (LLP) can be treated as one σ bond. Hybridization state of hetero atom along with the help of LLP in heterocyclic compounds has been shown in Table 1 below.

Table 1. (Hybridization state of hetero atom in heterocyclic compounds with the help of LLP)

Heterocyclic compounds	Number of σ bonds around hetero atom (from single and double bonds) (A)	LLP (localized lone pair of e⁻s) (B)	Total Number of σ bonds around hetero atom (A+B)	Power of the hybridization state of the hetero atom (corresponding hybridization state)
 Pyrrole	03	0 (lone pair of electron undergo delocalization with the ring system)	03	02 (sp^2 N)
 Furan	02	01 (out of two lone pair of electrons, one undergo delocalization and other remain as LLP)	03	02 (sp^2 O)
 Thiophene	02	01 (out of two lone pair of electrons, one undergo delocalization and other remain as LLP)	03	02 (sp^2 S)
 Pyridine	02	01	03	02 (sp^2 N)
 Indole	03	0	03	02 (sp^2 N)
 Quinoline	02	01	03	02 (sp^2 N)
 Isoquinoline	02	01	03	02 (sp^2 N)
 Imidazole	03 (N1) 02 (N3)	0 (N1) 01 (N3)	03 03	02 (sp^2 N1) 02 (sp^2 N3)

Heterocyclic compounds	Number of σ bonds around hetero atom (from single and double bonds) (A)	LLP (localized lone pair of e⁻s) (B)	Total Number of σ bonds around hetero atom (A+B)	Power of the hybridization state of the hetero atom (corresponding hybridization state)
 Pyrimidine	02 (N1) 02 (N3)	01 (N1) 01 (N3)	03 03	02 (sp^2 N1) 02 (sp^2 N3)
 Purine	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	02 (N) 02 (S)	01 (N) 01 (S) (out of two lone pair of electrons on S, one undergo delocalization and other remain as LLP)	03 03	02 (sp^2 N) 02 (sp^2 S)
 Benzothiazole	02 (N) 02 (S)	01 (N) 01 (S) (out of two lone pair of electrons on S, one undergo delocalization and other remain as LLP)	03 03	02 (sp^2 N) 02 (sp^2 S)

2. Aromaticity

It was first devised by Hückel in 1931. According to Hückel's rule of aromaticity, a molecule will be aromatic if it is a

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

Innovative Mnemonics on the Prediction of Aromatic behavior of Heterocyclic Compounds with DLP:

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

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.

Formula used for the prediction of 'A' value:

Evaluation of A Value:

$$\mathbf{A} = \pi\mathbf{b} + \mathbf{DLP} + \mathbf{1}(\mathbf{constant})$$

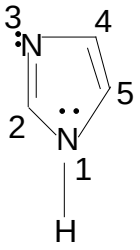
where, πb = number of π bonds with in the ring system;
DLP = Delocalized lone pair of electron.

For aromatic behavior of heterocyclic compounds A will be even number.

If a multi hetero atom based on the heterocyclic compound, containing both DLP and LLP hetero atoms, aromaticity should be predicted with respect to DLP based hetero atom only. But when both hetero atoms are in the same mode of classification (DLP or LLP) then aromaticity should be predicted with respect to that hetero atom which contains lowest possible position number as per IUPAC.

Eg. Imidazole 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.

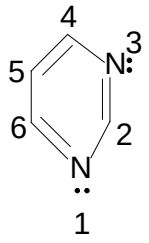
For N1, A = πb+DLP+1(constant) = 2+1+1 = 4 (even no) - Aromatic



Imidazole

Eg. Pyrimidine is a multi hetero atom based hetero cyclic compound in which, both N1 & N3 are in same environment (LLP based hetero atom) based hetero atom and N3 is LLP based hetero atom. In this case aromaticity should be predicted with respect to N1 (lowest possible position number).

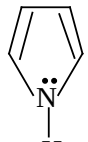
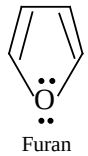
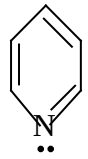
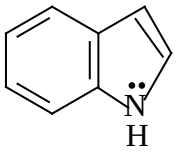
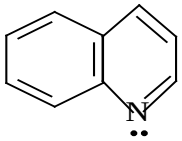
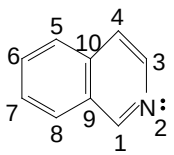
For N1, A = πb+DLP+1(constant) = 3+0+1 = 4 (even no) - Aromatic

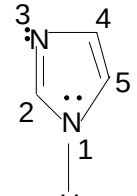
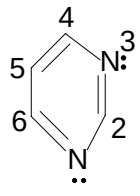
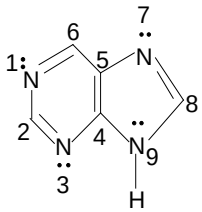
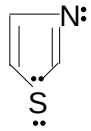
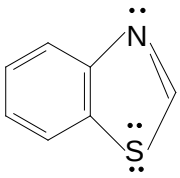


Pyrimidine

Aromaticity of heterocyclic compounds has been illustrated in Table 2.

Table 2. Aromatic behavior of heterocyclic compounds with the help of 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)	Nature of compound
 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 'S' 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

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)	Nature of compound
 Imidazole	02	01 (N1)	2 + 1 + 1 = 4 (even no)	Aromatic
 Pyrimidine	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

3. Conclusions

It might be expected that these two innovative mnemonics will help the students of chemical education at Undergraduate, Senior Undergraduate and Post-Graduate level to discriminate aromaticity and hybridization quite easily only by giving a look on the classification of lone pair of electrons (DLP or LLP). Experiment *in vitro* on 100 students showed that by using these formulae students can save up to 5-7 minutes time in the examination hall to find out the aromatic character and state hybridization for heterocyclic compounds. On the basis of this, I can strongly recommend to use these two time economic innovative mnemonics in the field of heterocyclic chemistry for a better comprehension and up gradation.

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In this special day (41th birth day – D.O.B.: 14/03/1978), I want to delegate my this innovative research article in the field of Chemical Education to my beloved father Late Anil Ranjan Das, who was a chemistry teacher and also founder of my chemistry life.

I would like to give my cordial thanks to Mr.Santanu Chakraborty, Lecturer, Department of English, Ramthakur College, Agartala, Tripura, for his helping manner in recasting statements in this article.

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