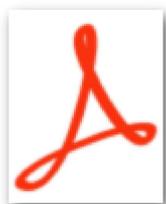# File:Chapter 2 - PREDICTION OF THE HYBRIDIZATION STATE OF ORGANIC COMPOUNDS pp 23-34.pdf

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## Summary

| | |
|---|---|
| **Description** | In this chapter 2, another formulae-based mnemonics by counting total number of σ bonds and localized negative charge (TSLNC) or localized lone pair of electrons (TSLLP) and subtract one (01) from this total value (TSLNC or TSLLP) to predict the power of the hybridization state of carbon atoms and hetero atoms in different organic compounds including heterocyclic compounds have been highlighted by innovative and time economic way. Educators can use this mnemonic in their teaching style in the classroom lectures after discussing conventional methods and its limitation to make chemistry intriguing. Here, I have tried to focus two (02) time economic mnemonics by including two (02) formulae for the prediction of hybridization of carbon atoms and hetero atoms in different organic compounds. This article encourages students to solve multiple choice type questions (MCQs) at different competitive examinations in a time economic ground on the prediction of hybridization state of carbon atoms and hetero atoms in different organic compounds. Prediction of hybridization state in different organic compounds is also useful to know the planarity of compounds, which is a very essential factor for evaluation of aromaticity of organic compounds. |
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# Chapter-2

## INNOVATIVE METHOD FOR THE PREDICTION OF THE HYBRIDIZATION STATE OF ORGANIC COMPOUNDS

### Arijit Das

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**In chapter1**, formulae based four mnemonics by counting total number of σ bonds and lone pair of electrons around the central atom and subtract one (01) from this total value ($T_{SLP}$) to predict the power of the hybridization state 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 hybridization state of simple molecules or ions.

**In this chapter 2**, another formulae-based mnemonics by counting total number of σ bonds and localized negative charge ($T_{SLNC}$) or localized lone pair of electrons ($T_{SLLP}$) and subtract one (01) from this total value ($T_{SLNC}$ or $T_{SLLP}$) to predict the power of the hybridization state of carbon atoms and hetero atoms in different organic compounds including heterocyclic compounds have been highlighted by innovative and time economic way. Educators can use this mnemonic in their teaching style in the classroom lectures after discussing conventional methods and its limitation to make chemistry intriguing.

Here, I have tried to focus two (02) time economic mnemonics by including two (02) formulae for the prediction of hybridization of carbon atoms and hetero atoms in different organic compounds. This article encourages students to solve multiple choice type questions (MCQs) at different competitive examinations in a time economic ground on the prediction of hybridization state of carbon atoms and hetero atoms in different organic compounds. Prediction of hybridization state in different organic compounds is also useful to know the planarity of compounds, which is a very essential factor for evaluation of aromaticity of organic compounds.

This chapter emphasizes chemical education in the light of other variety of mnemonics to make organic chemistry metabolic, time economic and intriguing for students because the use of mnemonics in classroom lectures is the very essential tool to become a distinguished educator. The conventional method on the prediction of hybridization state of carbon and heteroatoms in organic compounds to know the planarity of compounds is time-consuming [1-5].

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**1.** L. Pauling, "The Nature Chemical Bond. Application of Results Obtained from the Quantum Mechanics and from a Theory of Paramagnetic Susceptibility to the Structure of Molecules", *J.Am.Chem.Soc.* 53.4(1931): 1367-1400, doi:10.1021/ja01355a027, https://pubs.acs.org/doi/abs/10.1021%2Fja01355a027.
**2.** I.L. Finar, *Organic Chemistry 2* (Pearson: 2002), 606-637.
**3.** R.T. Morrison, and R.N. Boyd, *Organic Chemistry* (1992), 1059-1061.
**4.** T.W.Graham Solomons and C.B. Fryhle, *Organic Chemistry* (Wiley India: 2012), 655-658.
**5.** J.G. Smith, *Organic Chemistry* (2008), 616-619.

Keeping this in mind, in this book, I have introduced two innovative mnemonics to make this innovative pedagogical chapter 2 intriguing in all respect[6-10].

## METHODOLOGY

## 1.Classification of Negative Charge inorganic compounds

The negative charge on the carbon atom of any ring system can be generally classified into two types as delocalized negative charge (DNC) and localized negative charge (LNC) as follows:

a)**Delocalized negative charge (DNC):** When the negative charge on the carbon atom of the ring system of organic compounds undergo delocalization through conjugation then it is treated as delocalized negative charge (DNC). Negative charge bearing carbon atom of the ring system of an organic compound, when, directly attached with single bonds from all ends within the ring system, then it is considered as DNC containing carbon atom and its negative charge is to be treated as (DNC).

**Ex.** In cyclopropenyl anions, cyclopentadienyl anions and cycloheptatrienyl anions (**Fig. 2.14, Fig. 2.15, Fig. 2.16**) negative charge on C atom are to be treated as DNC, because, it is directly attached with single bonds directly from all side.
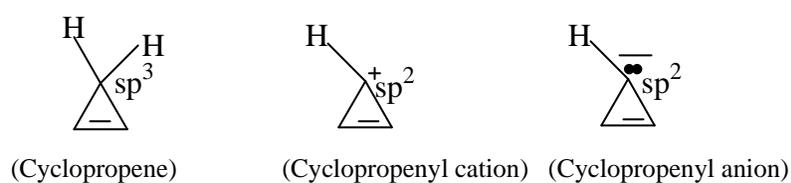


(Cyclopropene)    (Cyclopropenyl cation)  (Cyclopropenyl anion)

**Fig. 2.14: Structure of cyclopropene, cyclopropenyl cation, and cyclopropenyl anion**



(Cyclopentadienyl anion)    (Cyclopentadienyl cation)    (Cyclopentadiene)

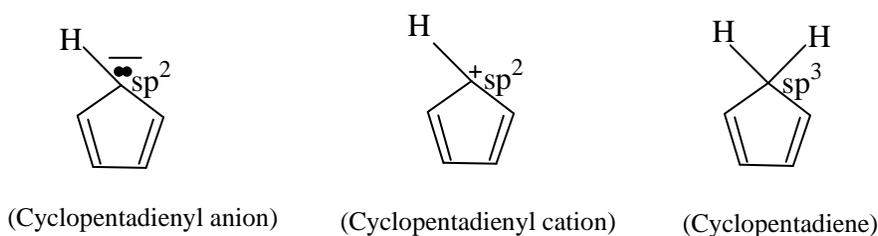**Fig. 2.15: Structure of cyclopentadienyl anion, cyclopentadienyl cation, and cyclopentadiene**

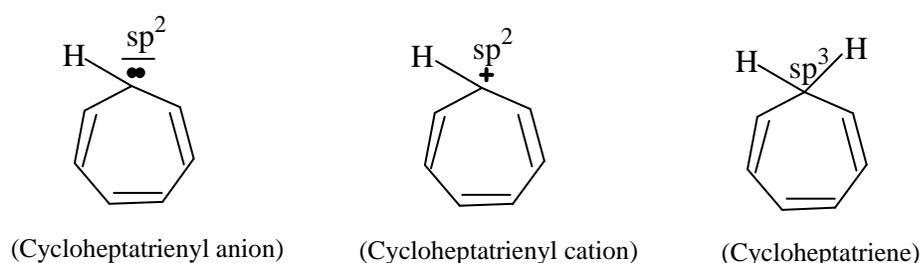(Cycloheptatrienyl anion)    (Cycloheptatrienyl cation)    (Cycloheptatriene)

**Fig. 2.16: Structure of cycloheptatrienyl anion, cycloheptatrienyl cation, and cycloheptatriene**

b) **Localized negative charge (LNC):** When the negative charge on the carbon atom of the ring system of organic compounds does not undergo delocalization through conjugation then it is to be treated as Localized negative charge (LNC). Negative charge bearing carbon atom of the ring system of an organic compound, when, directly attached with single and double bonds with the ring system is to be considered as LNC containing carbon atom and its negative charge is to be treated as localized negative charge (LNC).

**Ex.** In phenyl carbanion **(Figure 2.16a)** vertex carbon atom bearing a localized negative charge (LNC=1) is surrounded by 2σ bonds (one single bond and one double bond) around itself.
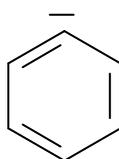


Fig. 2.16a. Structure of phenyl carbanion

## 2. Classification of Lone Pair of Electrons in heterocyclic compounds

Lone Pair of electrons can be generally classified into two types as Delocalized lone pair electron (DLP) and Localized lone pair electron (LLP) as follows[6-10] :

a) **Delocalized lone pair electron (DLP):** When the lone pair of electron of heteroatom undergo delocalization through conjugation then it is to be treated as a delocalized lone pair electron (DLP). The

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**6.** A. Das et.al, "A rapid and innovative method for the identification of aromatic and anti-aromatic nature of organic compounds", *World Journal of Chemical Education* 1 (Sept 2013): 6-8, doi: 10.12691/wjce-1-1-2, http://pubs.sciepub.com/wjce/1/1/2/# .
**7.** A. Das, "Innovative and Time Economic Pedagogical Views In Chemical Education - A Review Article", *World Journal of Chemical Education* 2 (July 2014): 29-38, doi:10.12691/wjce-2-3-1, http://pubs.sciepub.com/wjce/2/3/1/index.html#.
**8.** A. Das, "Lone Pair Electron Discriminate Hybridization with Aromatic and Anti Aromatic behavior of Heterocyclic Compounds - Innovative Mnemonics", *World Journal of Chemical Education* 6 (April 2018): 95-101, doi: 10.12691/wjce-6-2-4, http://pubs.sciepub.com/wjce/6/2/4/.
**9.** A. Das, "A Review of Time Economic Innovative Mnemonics In Chemical Education", *International Journal of Physics & Chemistry Education* 10, (June 2018): 27-40, doi: 10.12973/ijpce/81589, http://www.ijpce.org/A-Review-of-Time-Economic-Innovative-Mnemonics-in-Chemical-Education,81589,0,2.html.
**10.** A. Das, "Innovative Mnemonics In Chemical Education: Review Article", *African Journal of Chemical Education* 8, (July 2018): 144-189, https://www.ajol.info/index.php/ajce/article/view/176086.

The heteroatom (atom containing a lone pair electron), which is directly attached with single bonds only from all ends is to be considered as DLP based heteroatom and its lone pair is to be treated as (DLP).

**Ex.** In Pyrrole, (**Fig. 2.18**)**,** the lone pair of N atom is to be treated as DLP because it is directly attached with three single bonds only.

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

**Eg.** In Pyridine, (**Fig. 2.18**), the 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.
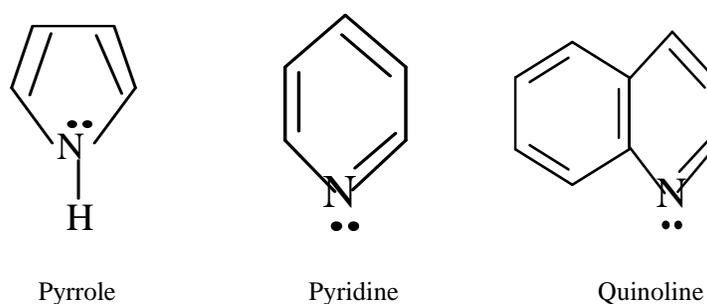


| Pyrrole | Pyridine | Quinoline |

**Fig. 2.18: Structure of pyrrole, pyridine, and quinoline**

### 3. Planarity of organic compounds

Planarity is one of the vital features for prediction aromatic, antiaromatic and nonaromatic behavior of heterocyclic compounds or other organic compounds. For aromatic and antiaromatic behavior the compound must be planar, whereas, the nonplanar compound is nonaromatic in nature. Planarity of heterocyclic compounds depends on the nature of the hybridization state of carbons and heteroatoms 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 nonplanar.

### 4. The conventional method for prediction of hybridization state organic compounds :

**Hybridization state for a molecule can be calculated by the formula P = 1/2 (V+MA−C+A),**

Where, V = Number of valance electrons in the central atom, MA = Number of surrounding monovalent atoms, C = Cationic charge, A = Anionic charge, P = power of the hybridization state of the central atom.

## 5. Innovative mnemonics for the prediction of hybridization state of carbon atom in organic compounds:

### Prediction of sp² and sp³ Hybridization state:

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

**Power on the Hybridization state of the heteroatom ($P_{Hyb}$) = ($T_{SLNC}$) − 1**

where, $P_{Hyb}$ = Power on the Hybridization state of the heteroatom, $T_{SLNC}$ = (Total no of σ bonds around each central atom + LNC), LNC = Localized negative charge.

All single (-) bonds are the σ bond, in a double bond (=) there is one σ and one π. 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.

## 6. Innovative mnemonics for prediction of the hybridization state of the heteroatom in different heterocyclic compounds:

### Prediction of sp² and sp³ Hybridization state:

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

**Power on the Hybridization state of the heteroatom ($P_{Hyb}$) = ($T_{SLLP}$) − 1**

where, $P_{Hyb}$ = Power on the Hybridization state of the heteroatom, $T_{SLLP}$ = (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 the σ bond, in a double bond (=) there is one σ and one π.

## RESULTS AND DISCUSSION

## 1. Innovative mnemonics for prediction of the hybridization state (sp² & sp³) of carbon atom in organic compounds can be well explained in the following way:

Hybridization state of carbon atom in organic compounds can be calculated from the total number of σ bonds around carbon atom and number of localized negative charge ($T_{SLNC}$) on the carbon atom and subtract one (01) from this total value of $T_{SLNC}$ to get the hybridization state ($sp^2$ & $sp^3$) of the carbon atom in the organic compounds.

**Ex.a.** In cyclopropene, cyclopentadiene and cycloheptatriene (**Fig.2.14, Fig.2.15, Fig.2.16),** vertex carbon atom is in $sp^3$ hybridization state. Here in all cases, the vertex carbon atom is surrounded by 4 single bonds ($\sigma$ bonds) around itself, hence, power of the hybridization state, $(P_{Hyb})$ = $(T_{SLNC}) - 1 = 4\text{-}1 = 3$ ($sp^3$), whereas, rest carbon atoms bearing $sp^2$ hybridization state corresponding to $3\sigma$ bonds (2 single bonds and one double bond) around themselves. The presence of one $sp^3$ hybridized carbon atom along with other $sp^2$ hybridized carbons makes cyclopropene, cyclopentadiene, and cycloheptatriene nonplanar.

**Ex.b.** In cyclopropenyl anions, cyclopentadienyl anions and cycloheptatrienyl anions (**Fig. 2.14, Fig. 2.15, Fig. 2.16),** vertex carbon atom bearing a negative charge are in $sp^2$ hybridization state. Here in all cases, the vertex carbon atom is surrounded by 3 single bonds ($\sigma$ bonds) around itself, because, here, the negative charge of the vertex carbon atom is treated as delocalized negative charge (DNC) and cannot be counted during prediction of the hybridization state of the vertex carbon atom. Hence, the power of the hybridization state, $(P_{Hyb}) = (T_{SLNC}) - 1 = 3\text{-}1 = 2$ ($sp^2$), whereas, rest carbon atoms also bear $sp^2$ hybridization state corresponding to $3\sigma$ bonds (2 single bonds and one double bond). The presence of all $sp^2$ hybridized carbons in cyclopropenyl anions, cyclopentadienyl anions, and cycloheptatrienyl anions make them planar.

**Ex.c.** In cyclopropenyl cations, cyclopentadienyl cations and cycloheptatrienyl cations (**Fig. 2.14, Fig. 2.15, Fig. 2.16),** vertex carbon atom bearing a positive charge are in $sp^2$ hybridization state. Here in all cases, the vertex carbon atom is surrounded by 3 single bonds ($\sigma$ bonds) around itself. Hence, the power of the hybridization state, $(P_{Hyb})$ = $(T_{SLNC}) - 1 = 3\text{-}1 = 2$ ($sp^2$), whereas, rest carbon atoms also bear $sp^2$ hybridization state corresponding to $3\sigma$ bonds (2 single bonds and one double bond). The presence of all $sp^2$ hybridized carbons in cyclopropenyl cations, cyclopentadienyl cations, and cycloheptatrienyl cations make them planar.

**Ex.d.** In cyclobutadiene and cyclooctatetraene (**Fig. 2.17),** all carbon atoms are surrounded by $3\sigma$ bonds (2 single bonds and one double bond), hence, the power of the hybridization state, $(P_{Hyb})$ = $(T_{SLNC}) - 1 = 3\text{-}1 = 2$ ($sp^2$), which makes them planar.
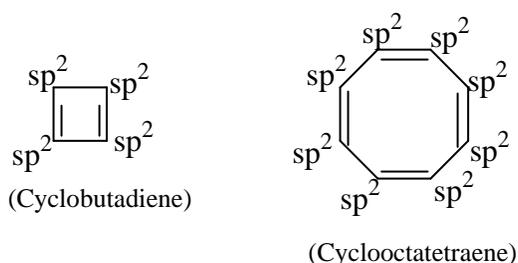


(Cyclobutadiene)

(Cyclooctatetraene)

**Fig. 2.17: Structure of Cyclobutadiene and Cyclooctatetraene**

## 2. Innovative mnemonics for the prediction of the hybridization state ($sp^2$ & $sp^3$) of the heteroatom in heterocyclic compounds can be well explained in the following way:

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

**Ex.a.** In Pyridine **(Fig.2.18)**, lone pair of 'N' atom is to be treated as localized lone pair of electron (LLP), because, it is directly attached with double and single bonds with the ring system, hence, it is considered for calculating the power of the hybridization state, ($P_{Hyb}$) = ($T_{SLLP}$) − 1, to predict the hybridization state of heteroatom 'N' in pyridine. Here, in pyridine, around 'N', there are two σ bonds and one LLP (localized lone pair electrons). Hence, power of the hybridization state of 'N' in pyridine, ($P_{Hyb}$) = ($T_{SLLP}$) − 1 = (2+1)-1 = 2 ($sp^2$-N). All rest five carbon atoms are in same hybridization state $sp^2$, hence, pyridine is planar.

**Ex.b.** In Pyrrole **(Fig.2.18)**, the lone pair of N atom is to be treated as DLP (delocalized lone pair electron - lone pair electron of heteroatom which is directly attached with single bonds only from all ends with the ring system), because, it is directly attached with three single bonds only. Hence, is not to be under consideration for calculating the power of the hybridization state, ($P_{Hyb}$) = ($T_{SLLP}$) − 1, to predict the hybridization state of heteroatom 'N' in pyrrole. Here, in pyrrole, around 'N', there are three σ bonds and zero LLP (localized lone pair electrons). Hence, power of the hybridization state of 'N' in pyrrole, ($P_{Hyb}$) = ($T_{SLLP}$) − 1 = (3+0)-1 = 2 ($sp^2$-N). All rest four carbon atoms are in same hybridization state $sp^2$, hence, pyrrole is planar.

**Ex.c.** In quinoline **(Fig.2.18)**, lone pair of 'N' atom is to be treated as localized lone pair of electron (LLP), because, it is directly attached with double and single bonds with the ring system, hence, it is considered for calculating the power of the hybridization state, ($P_{Hyb}$) = ($T_{SLLP}$) − 1, to predict the hybridization state of heteroatom 'N' in quinoline. Here, in quinoline, around 'N', there are two σ bonds and one LLP (localized lone pair electrons). Hence, power of the hybridization state of 'N' in quinoline, ($P_{Hyb}$) = ($T_{SLLP}$) − 1 = (2+1)-1 = 2 ($sp^2$-N). All rest carbon atoms are in same hybridization state $sp^2$, hence, quinoline is planar. **Ex.d.** In, aziridine **(Fig.2.19)**, 'N' atom is surrounded by three σ bonds and one LLP (localized lone pair electrons).

Hence, power of the hybridization state of 'N' in aziridine, $(P_{Hyb}) = (T_{SLLP}) - 1 = (3+1)-1 = 3$ (sp³-N). Hence, it is non planar.
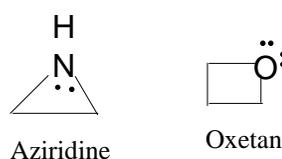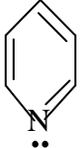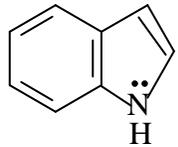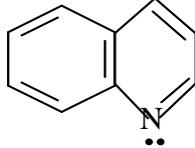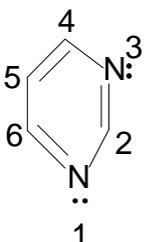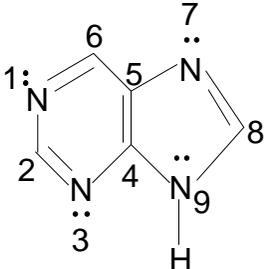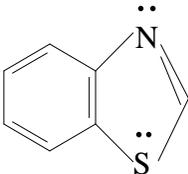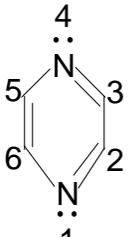


Aziridine   Oxetan

**Fig.2.19: Structure of aziridine and oxetan**
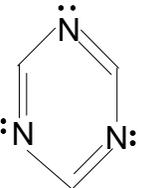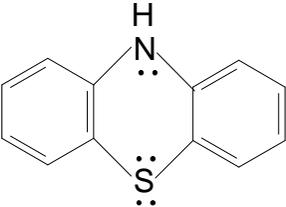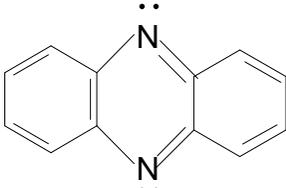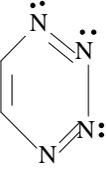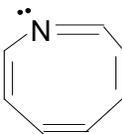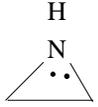
Adequate examples on prediction of the hybridization state of heteroatom in heterocyclic compounds containing one, two or more same or different number of heteroatoms from the corresponding $T_{SLLP}$ value (total number of σ bonds around the central atom + localized lone pair of electrons on the central atom) of the central atom have been explored in (**Table 2.3**).
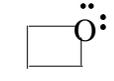
## Table-2.3 Hybridization state of Heteroatom in Heterocyclic Compounds with the help of LLP

| Heterocyclic Compounds (Planar/nonplanar) | Number of σ bonds around the hetero atom (from single and double bonds) ($T_S$) | Number of localized Lone Pair of e⁻s (LLP) | Total Number of σ bonds around the hetero atom ($T_{SLLP}$) | Power on the Hybridization state of the heteroatom $(P_{Hyb}) = (T_{SLLP}) - 1$ (Corresponding Hybridization state) |
|---|---|---|---|---|
| Pyrrole (Planar) | 03 | 0 (the lone pair of electron undergo delocalization, DLP with the ring system) | 03 | 02 (sp² N) |
| Furan (Planar) | 02 | 01 (out of two lone pairs of electrons, one undergo delocalization, DLP and other remain as LLP) | 03 | 02 (sp² O) |
| Thiophene (Planar) | 02 | 01 (out of two lone pairs of electrons of S one undergo delocalization, DLP and other remain as LLP) | 03 | 02 (sp² S) |

| Structure | | | | |
|---|---|---|---|---|
| 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) | 01 (N1) | 03 | 02 (sp² N1) |
| | 02 (N3) | 01 (N3) | 03 | 02 (sp² N3) |
| | 02 (N7) | 01 (N7) | 03 | 02 (sp² N7) |
| | 03 (N9) | 0 (N9) | 03 | 02 (sp² N9) |
| Thiazole (Planar) | 02 (N) | 01 (N) | 03 | 02 (sp² N) |
| | 02 (S) | 01 (S) (out of two lone pairs of electrons on S, one undergo delocalization, DLP and other remain as LLP) | 03 | 02 (sp² S) |
| Benzothiazole (Planar) | 02 (N) | 01 (N) | 03 | 02 (sp² N) |
| | 02 (S) | 01 (S) (out of two lone pairs of electrons on S, one undergo delocalization, DLP and other remain as LLP) | 03 | 02 (sp² S) |
| Pyrazine (p-diazine) (Planar) | 02 (N1) | 01 (N1) | 03 | 02 (sp² N1) |
| | 02 (N1) | 01 (N1) | 03 | 02 (sp² N4) |

| | | | | |
|---|---|---|---|---|
| Cyanidine (Planar) | 02 (N1, N3, and N5) | 01 (N1, N3, and N5) | 03 | 02 (sp² N1,N3,N5) |
| Phenothiazine (Planar) | 03 (N) <br><br> 02 (S) | 0 (N) <br><br> 01 (S) (out of two LP of S, one undergo delocalization(DLP), and others remain as LLP) | 03 <br><br> 03 | 02 (sp² N) <br><br> 02 (sp² S) |
| Phenazine (Planar) | 02 (both N) | 01 (both N) | 03 | 02 (sp² both N) |
| 1,2,3,4-tetrazine (Planar) | 02 (N1,N2,N3,N4) | 01 (N1,N2,N3,N4) | 03 | 02 (sp² All N) |
| Azocine (Planar) | 02 | 01 | 03 | 02 (sp² N) |
| Azetine (Planar) | 02 | 01 | 03 | 02 (sp² N) |
| Aziridine (non-planar) | 03 | 01 | 04 | 03 (sp³ N) |

| | | | | |
|---|---|---|---|---|
| $\boxed{\ddot{O}\!:}$ <br> Oxetan <br> (non-planar) | 02 | 02 | 04 | 03 <br> (sp$^3$ O) |
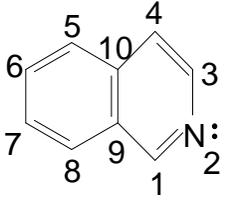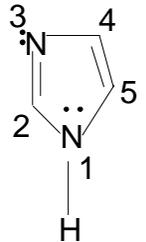
## Conclusion

It may be expected that this time economic innovative methodology, described in chapter 2, will help the student of chemical education at Undergraduate, Senior Undergraduate and Post-Graduate level to **predict hybridization state of carbon atoms and hetero atom in organic compounds** which will be **helpful to detect planarity and aromaticity of organic compounds.** Experiments, *in vitro,* on 100 students, showed that, **by using these innovative formulae, students can save up to 2-3 minutes' time in the examination hall** to find out the hybridization state of carbon atoms and hetero atoms in organic compounds. **On the basis of this, I can strongly recommend using these time economic innovative mnemonics in organic chemistry.**

## Contributor:

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