

## Predicting the hybridization state: a comparative study between conventional and innovative formulae

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### ABSTRACT

In previous published articles, formulae-based mnemonics by counting the total number of  $\sigma$  bonds with a lone pair of electrons (LP), a localized negative charge (LNC), or a localized lone pair of electrons (LLP) and subtracting one (01) from this total value ( $T_{SLP}$ ,  $T_{SLNC}$ , or  $T_{SLLP}$ ) to predict the power of the hybridization state of simple molecules or ions and organic compounds, including heterocyclic compounds have been discussed. These are the innovative and time-efficient methods of enhancing student interest. Here, in this new article, the limitations of conventional formulae in comparison to the use of innovative formulae have been discussed along with the application of the hybridization state in different fields of chemical education. 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 simple molecules or ions to know their normal and subnormal geometry and prediction of hybridization state of hetero atom in different heterocyclic compounds to know the planarity of the compounds, which is very essential factor for prediction of aromaticity of heterocyclic compounds. Educators can use this comparative study in their classroom lectures to make chemistry authentic and intriguing. Because the use of mnemonics in classroom lectures is an essential tool to become a distinguished educator.

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## 1. INTRODUCTION

Conventional formulae by using conventional methods [1-20] for the prediction of hybridization state of simple molecules or ions, organic compounds including different heterocyclic compounds containing one, two or more number of hetero atoms is mystifying and time consuming. Keeping this in mind, I have introduced formulae-based mnemonics by counting the total number of  $\sigma$  bonds with a lone pair of electrons (LP), a localized negative charge (LNC), or a localized lone pair of electrons (LLP) and subtracting one (01) from this total value ( $T_{SLP}$ ,  $T_{SLNC}$ , or  $T_{SLLP}$ ) to predict the power of the hybridization state of simple molecules or ions and organic compounds, including heterocyclic compounds [21-27].

Conventional formula for the prediction of hybridization state of simple molecules or ions and hetero atom in different heterocyclic compounds had wide limitations in the field of both organic and inorganic chemistry which were misguided by the educators since last 80-90 years. In this article, I have tried to focus the limitations of conventional formula to predict the hybridization state of center atom in simple molecules or ions and also in the organic compounds in and solved them in the light of innovative formulae.

## 2. FORMULAE BASED METHODOLOGIES

### 2.1. Conventional formulae

*Conventional formulae* using conventional methods [1-20] for the prediction of the hybridization state:

The hybridization state for a molecule can be calculated using  $P = 1/2 (V + MA - C + A)$ , where  $V$  = the number of valance electrons in the central atom,  $MA$  = the number of surrounding monovalent atoms,  $C$  = cationic charge,  $A$  = anionic charge, and  $P$  = power of the hybridization state.

### 2.2. Innovative formulae-1

**An innovative formula [21-23, 25-27] for predicting the hybridization state of simple molecules or ions:**

The power of the hybridization state of the central atom is  $(P_{\text{Hyb}}) = (T_{\text{SLP}}) - 1$ ,

Where  $P_{\text{Hyb}}$  = power of the hybridization state of the central atom,  $T_{\text{SLP}}$  = (total number of  $\sigma$  bonds around each central atom + LP).

In order to work out a molecule's Lewis structure, first predict the number of sigma bonds ( $\sigma$ -bonds), pi bonds ( $\pi$ -bonds), and the lone pair of electrons (LP), if any. All single (-) bonds are  $\sigma$  bonds, while  $1\sigma$  and  $1\pi$  are the double bond (=), and  $1\sigma$  and  $2\pi$  (exclude  $\pi$  bond) form the triple bond ( $\equiv$ ). In addition to these, each co-ordinate bond ( $\rightarrow$ ) can be treated as a  $1\sigma$  bond. This formula is applicable up to four (04) $T_{\text{SLP}}$ .

If the power of the hybridization state ( $P_{\text{Hyb}}$ ) is 03, 02, and 01 then the hybridization state will be  $sp^3$ ,  $sp^2$ , and  $sp$ , respectively.

### 2.3. Innovative formulae-2

An innovative formula [21-27] for predicting the hybridization state of carbon atom in different organic compounds:

Power of the hybridization state in the central atom,  $(P_{\text{Hyb}}) = (T_{\text{SLNC}}) - 1$

Where  $P_{\text{Hyb}}$  = power of the hybridization state of the central atom, and  $T_{\text{SLNC}}$  = (total number of  $\sigma$  bonds around each central atom + localized negative charge).

All single (-) bonds are  $\sigma$  bonds, while  $1\sigma$  and  $1\pi$  are the double bond (=). Also, (LNC) = localized negative charge. A negative charge bearing carbon atom in the ring system of the organic compound when directly attached with single and double bonds is considered to be an LNC containing carbon atom and its negative charge is to be treated accordingly.

### 2.4. Innovative formulae-3

An innovative formula [22-24] for predicting the hybridization state of the heteroatom in different heterocyclic compounds:

Power of the hybridization state of a heteroatom  $(P_{\text{Hyb}}) = (T_{\text{SLLP}}) - 1$ ,

Where  $P_{\text{Hyb}}$  = power of the hybridization state of the heteroatom,  $T_{\text{SLLP}}$  = (total number of  $\sigma$  bonds around each central atom + LLP), and LLP = localized lone pair of electrons. If the power of the hybridization state ( $P_{\text{Hyb}}$ ) is 03, 02, and 01 then the hybridization state will be  $sp^3$ ,  $sp^2$ , and  $sp$ , respectively. All single (-) bonds are  $\sigma$  bonds, while in a double bond (=) there is one  $\sigma$  and one  $\pi$ . The heteroatom (an atom containing a lone pair of electrons), which is directly attached with single and double bonds using the ring system, is considered to be an LLP-based heteroatom and its lone pair is to be treated as a localized lone pair of electrons (LLP).

## 3. RESULTS AND ANALYSIS

### 3.1. Comparative study between conventional and innovative formulae for the prediction of the hybridization state of different atoms in simple molecules or ions.

When using a conventional formula, it is not possible to predict the hybridization state of an O atom in the cyclic ozone, as illustrated in Figure 1

**Example 1:** The hybridization state of O in cyclic ozone

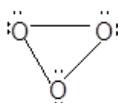


Figure 1. Equilateral triangle structure of cyclic ozone ( $O_3$ )

Conventional formula:  $P = 1/2 (V+MA-C+A) = 1/2 (6+0-0) = 3.0$  ( $sp^2$ - erroneous hybridization state of O)

Innovative formula:  $(P_{Hyb}) = (T_{SLP}) - 1 = (2+2)-1 = 3$  ( $sp^3$  hybridized O atom in cyclic ozone)

Where  $P_{Hyb}$  = power of the hybridization state of the central atom, and  $T_{SLP}$  = (total number of  $\sigma$  bonds around each central atom + LP)

It is not possible to predict the hybridization state of the S atom in  $S_8$  and the P atom in  $P_4$  using a conventional formula, as shown in Figure 2.

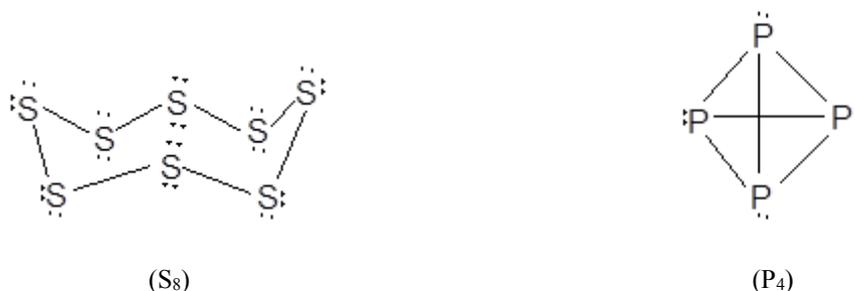


Figure 2. Zig-zag structure of  $S_8$  and Tetrahedron structure of  $P_4$

**Example 2:** The hybridization state of S in  $S_8$

Conventional formula:  $P = 1/2 (V+MA-C+A) = 1/2 (6+0-0) = 3.0$  ( $sp^2$ - erroneous hybridization state of S in  $S_8$ )

Innovative formula:  $(P_{Hyb}) = (T_{SLP}) - 1 = (2+2)-1 = 3$  ( $sp^3$  hybridized S atom in  $S_8$ )

Where  $P_{Hyb}$  = power of the hybridization state of the central atom, and  $T_{SLP}$  = (total number of  $\sigma$  bonds around each central atom + LP)

**Example 3:** The hybridization state of P in  $P_4$

Conventional formula:  $P = 1/2 (V+MA-C+A) = 1/2 (5+0-0) = 2.5$  (unpredictable hybridization state of P in  $P_4$ )

Innovative formula:  $(P_{Hyb}) = (T_{SLP}) - 1 = (3+1)-1 = 3$  ( $sp^3$  hybridized P atom in  $P_4$ ),

Where  $P_{Hyb}$  = power of the hybridization state of the central atom,  $T_{SLP}$  = (total number of  $\sigma$  bonds around each central atom + LP)

It is not possible to predict the hybridization state of a terminal carbon atom in alkynes using a conventional formula.

**Example 4:** The hybridization state of Ethyne, as presented in Figure 3.

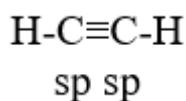


Figure 3. Linear structure of Ethyne ( $C_2H_2$ )

Conventional formula:  $P = 1/2 (V+MA-C+A) = 1/2 (4+1-0) = 2.5$  (unpredictable hybridization state).

Innovative formula:  $(P_{Hyb}) = (T_{SLP}) - 1 = 2-1 = 1$  ( $sp$  hybridized carbon atom in alkyne),

where  $P_{Hyb}$  = power of the hybridization state of the central atom,  $T_{SLP}$  = (total number of  $\sigma$  bonds around each central atom + LP)

**Example 5:** The hybridization state of pent-1-ene-4-yne, as presented in Figure 4.

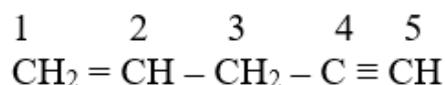


Figure 4. Structure of pent-1-ene-4-yne

Conventional formula: power of the hybridization state of the terminal carbon

$$C_5(P) = 1/2 (V+MA-C+A) = 1/2 (4+1-0) = 2.5 \text{ (unpredictable hybridization state } C_5).$$

Innovative formula: ( $P_{Hyb}$ ) for  $C_5 = (T_{SLP}) - 1 = 2 - 1 = 1$  (sp hybridized  $C_5$ ),

Where  $P_{Hyb}$  = power of the hybridization state of the central atom,  $T_{SLP}$  = (total no of  $\sigma$  bonds around each central atom + LP)

It is not possible to predict the hybridization state of oxygen atoms in the cyclic ozone or hydrogen peroxide, the S atom in  $S_8$ , or the P atom in  $P_4$  using a conventional formula; however, using an innovative formula allows the hybridization state to be determined with absolute accuracy in all cases.

### 3.2. A comparative study between conventional and innovative formulae to predict the hybridization state of carbon atoms in different non-heterocyclic organic compounds

It is not possible to predict the hybridization state of carbon atoms in cyclopropene, cyclopentadiene, cycloheptatriene, cyclopropenyl anion, cyclopentadienyl anion, cycloheptatrienyl anion, cyclopropenyl cation, cyclopentadienyl cation, and cycloheptatrienyl cation, benzene, and toluene using a conventional formulae; however, using an innovative formula allows the hybridization state to be determined with absolute accuracy in all cases.

When a conventional formula was used the hybridization state of a vertex carbon atom in cycloalkenes, such as cyclopropene, cyclopentadiene, and cycloheptatriene, as shown in Figure 5, Figure 6, and Figure 7, it gave erroneous results.

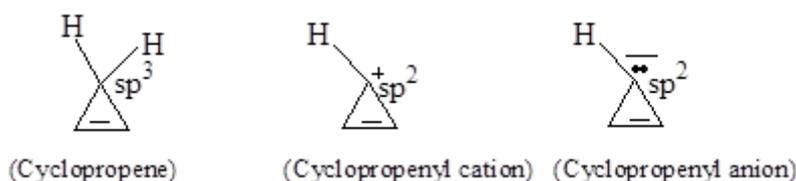


Figure 5. Structure of cyclopropene, cyclopropenyl cation, and cyclopropenyl anion

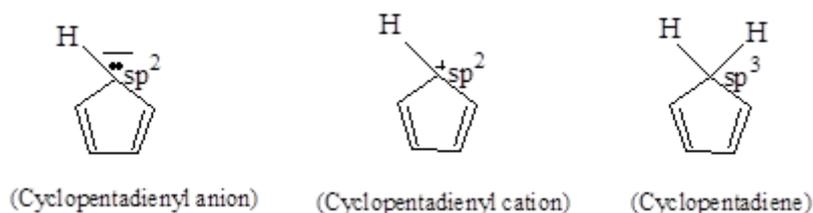


Figure 6. Structure of cyclopentadienyl anion, cyclopentadienyl cation, and cyclopentadiene

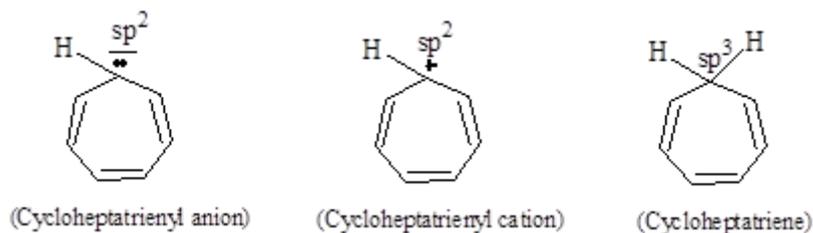


Figure 7. Structure of cycloheptatrienyl anion, cycloheptatrienyl cation, and cycloheptatriene

#### i) Conventional formula

The power of the hybridization state of the vertex carbon ( $P$ ) =  $1/2 (V+MA-C+A) = 1/2 (4+2-0) = 3$  ( $sp^2$ - erroneous hybridization state).

#### ii) Innovative formula

Power of the hybridization state, ( $P_{Hyb}$ ) =  $(T_{SLNC}) - 1 = 4 - 1 = 3$  ( $sp^3$  hybridization state of vertex carbon).

The hybridization state of carbon atoms, other than vertex carbon, in cycloalkenes, such as cyclopropene, cyclopentadiene and cycloheptatriene, Figure 5, Figure 6, and Figure 7, was unpredictable when using a conventional formula.

i) Conventional formula

The power of the hybridization state of the rest carbons ( $P$ ) =  $1/2 (V+MA-C+A)$  =  $1/2 (4+1-0)$  = 2.5 (unpredictable hybridization state).

ii) Innovative formula

The power of the hybridization state was ( $P_{Hyb}$ ) = ( $T_{SLNC}$ ) - 1 = 3-1 = 2 (sp<sup>2</sup> hybridization state of rest carbons other than vertex carbon).

The hybridization state of vertex carbon atoms bearing a negative charge in cycloalkenyl anions, such as cyclopropenyl anion, cyclopentadienyl anion, and cycloheptatrienyl anion, Figure 5, Figure 6, and Figure 7, was erroneous when using a conventional formula.

i) Conventional formula

The power of the hybridization state of the vertex carbon ( $P$ ) =  $1/2 (V+MA-C+A)$  =  $1/2 \{4+1-(0-1)\}$  =  $1/2 \{6\}$  = 3 (sp<sup>2</sup> - erroneous hybridization state).

ii) Innovative formula

The power of the hybridization state of the vertex carbon is ( $P_{Hyb}$ ) = ( $T_{SLNC}$ ) - 1 = 3-1 = 2 (sp<sup>2</sup> hybridization state).

The hybridization state of a vertex carbon atom bearing a positive charge in cycloalkenyl cations, such as cyclopropenyl cation, cyclopentadienyl cation, and cycloheptatrienyl cation, Figure 5, Figure 6, and Figure 7, was erroneous when using a conventional formula.

i) Conventional formula

The power of the hybridization state in a vertex carbon bearing a positive charge, ( $P$ ) =  $1/2 (V+MA-C+A)$  =  $1/2 \{4+1-(1+0)\}$  =  $1/2 \{4\}$  = 2 (sp - erroneous hybridization state).

ii) Innovative formula

Power of the hybridization state of the vertex carbon bearing positive charge, ( $P_{Hyb}$ ) = ( $T_{SLNC}$ ) - 1 = 3-1 = 2 (sp<sup>2</sup> hybridization state).

The hybridization state of carbon atoms in benzene, toluene, and so on is unpredictable using a conventional formula but, when using an innovative formula, the hybridization state will be determined with absolute accuracy in all cases.

A carbon atom in benzene as illustrated in Figure 8

i) Conventional formula

The power of the hybridization state of carbon is ( $P$ ) =  $1/2 (V+MA-C+A)$  =  $1/2 (4+1-0)$  = 2.5 (unpredictable hybridization state).

ii) Innovative formula

The power of the hybridization state of a carbon atom is ( $P_{Hyb}$ ) = ( $T_{SLNC}$ ) - 1 = 3-1 = 2 (sp<sup>2</sup> hybridization state).

Carbon atom from the methyl group in Toluene as illustrated in Figure 8

i) Conventional formula

The power of the hybridization state of a carbon atom from the methyl group in toluene is ( $P$ ) =  $1/2 (V+MA-C+A)$  =  $1/2 (4+3-0)$  = 3.5 (unpredictable hybridization state).

ii) Innovative formula

The power of the hybridization state of a carbon atom from the methyl group in toluene is ( $P_{Hyb}$ ) = ( $T_{SLNC}$ ) - 1 = 4-1 = 3 (sp<sup>3</sup> hybridization state).

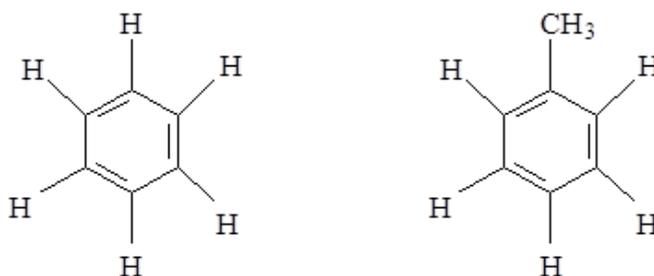


Figure 8. Structure of benzene and toluene

### 3.3. A comparative study between conventional and innovative formulae to predict the hybridization state of a heteroatom in different heterocyclic compounds

It is not possible to predict the hybridization state of heteroatom nitrogen in pyridine, quinoline, isoquinoline, pyrimidine, thiazole, benzothiazole, pyrazine, cyanidine, phenazine, 1,2,3,4-tetrazine, azocine, azetine, and aziridine, or an oxygen atom in oxetan using a conventional formula. However, when using an innovative formula, the hybridization state of a heteroatom in nitrogen will be determined with absolute accuracy in all cases.

#### i) Conventional formula

The power of the hybridization state of a nitrogen atom in pyridine is  $P = 1/2 (V+MA-C+A) = 1/2 (5 + 0 - 0 + 0) = 2.5$  (unpredictable hybridization state) and the power of the hybridization state of a nitrogen atom in quinoline is  $P = 1/2 (V+H-C+A) = 1/2 (5 + 0 - 0 + 0) = 2.5$  (unpredictable hybridization state) illustrated in Figure 9.

The power of the hybridization state of a nitrogen atom in aziridine is  $P = 1/2 (V+MA-C+A) = 1/2 (5 + 1 - 0 + 0) = 3$  ( $sp^2$ - erroneous hybridization state of N) and the power of the hybridization state of an oxygen atom in oxetan is  $P = 1/2(V+MA-C+A) = 1/2 (6 + 0 - 0 + 0) = 3$  ( $sp^2$ - erroneous hybridization state of oxygen atom) illustrated in Figure 10.

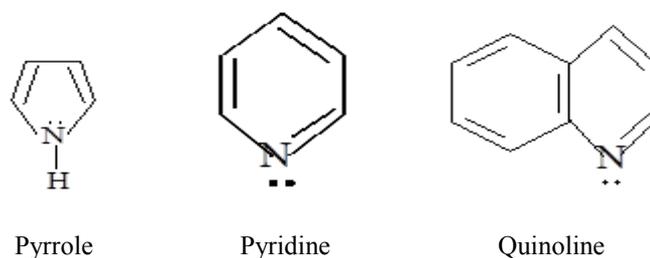


Figure 9. Structure of pyrrole, pyridine, and quinoline

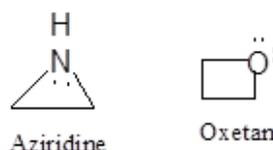


Figure 10. Structure of aziridine and oxetan

#### ii) Innovative formula

The power of the hybridization state of a heteroatom is  $(P_{Hyb}) = (T_{SLLP}) - 1$ .

The power of the hybridization state of a nitrogen atom in pyridine is  $P_{Hyb} = (3 - 1) = 2$  ( $\sigma$  bonds = 2 & LLP = 1)

( $sp^2$  hybridization state of N atom) and the power of the hybridization state of a nitrogen atom in quinoline is  $P_{Hyb} = (3 - 1) = 2$  ( $\sigma$  bonds = 2 & LLP = 1) ( $sp^2$  hybridization state of N atom) illustrated in Figure 9.

The power of the hybridization state of a nitrogen atom in aziridine is  $P_{Hyb} = (4 - 1) = 3$  ( $\sigma$  bonds = 3 & LLP = 1)

( $sp^3$  hybridization state of N atom) and the power of the hybridization state of an oxygen atom in oxetan is  $P_{Hyb} = (4 - 1) = 3$  ( $\sigma$  bonds = 2 & LLP = 2) ( $sp^3$  hybridization state of O atom) illustrated in Figure 10.

## 4. CONCLUSION

In this article, the limitations of conventional formulae have been discussed in the light of innovative formulae to predict the hybridization state of simple molecules or ions and organic compounds, including heterocyclic compounds. Educators can use this comparative study in their classroom lectures to make chemistry intriguing and trustworthy.

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