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Summary

Description	In the previous two chapters (chapter 1 & 2), formulae based mnemonics by counting total number of σ bonds with lone pair of electrons (LP) or localized negative charge (LNC) or localized lone pair of electrons (LLP) and subtract one (01) from this total value (TSLP , TSLNC or TSLLP) to predict the power of the hybridization state of simple molecules or ions and organic compounds including heterocyclic compounds 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 and organic compounds including heterocyclic compounds. But in this chapter, limitation of conventional formula and its comparative study in the light of innovative formulae have been discussed. Educators can use this comparative study in their teaching style in the classroom lectures to make chemistry intriguing.
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Chapter-3

Prediction Of The Hybridization State – A Comparative Study Between Conventional And Innovative Formulae

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In the previous two chapters (chapter 1 & 2), formulae based mnemonics by counting total number of σ bonds with lone pair of electrons (LP) or localized negative charge (LNC) or localized lone pair of electrons (LLP) and subtract 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 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 and organic compounds including heterocyclic compounds. But in this chapter, limitation of conventional formula and its comparative study in the light of innovative formulae have been discussed. Educators can use this comparative study in their teaching style in the classroom lectures to make chemistry intriguing.

FORMULAE

i) Conventional formulae for prediction of hybridization state

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.

ii) An innovative formula for predicting hybridization state of 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.

iii) An innovative formula for predicting hybridization state of carbon atom in different organic compounds:

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

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

All single (-) bonds are the σ bond, in the double bond (=), there is 1σ and 1π. (LNC) = Localized negative charge. Negative charge bearing carbon atom in the ring system of the 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).

iv)An innovative formula for predicting hybridization state of the heteroatom in different heterocyclic compounds:

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. The heteroatom (atom containing a 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).

RESULTS AND DISCUSSION

A. Comparative study between conventional and innovative formula for prediction of hybridization state of different atoms in simple molecules or ions

By using conventional formula it is not possible for the prediction of hybridization state of O atom in cyclic ozone (**Fig. 1.2)** as follows:

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

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

where, P_{Hyb} = Power on the Hybridization state of the central atom, T_{SLP} = (Total no of σ bonds around each central atom + LP)

By using conventional formula it is not possible for the prediction of hybridization state of S atom in S_8 and P atom in P_4 **(Fig. 1.4)** as follows:

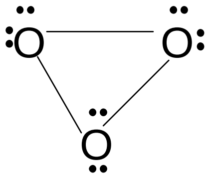
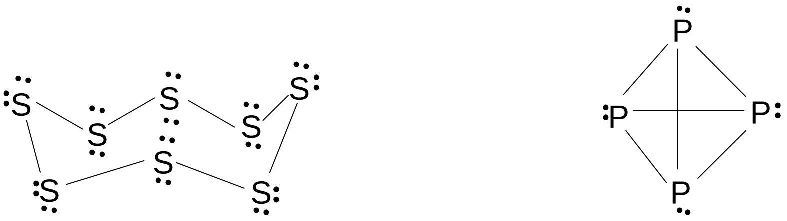


Fig. 1.2. Equilateral triangle structure of cyclic ozone (O_3)



(S_8) **(P_4)**

Fig. 1.4. Zig-zag structure of S_8 and Tetrahedron structure of P_4

Ex.1. Hybridization state of S in S_8

By 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)

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

where, P_{Hyb} = Power on the Hybridization state of the central atom, T_{SLP} = (Total no of σ bonds around each central atom + LP)

Ex.2. Hybridization state of P in P_4

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

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

where, P_{Hyb} = Power on the Hybridization state of the central atom, T_{SLP} = (Total no of σ bonds around each central atom + LP)

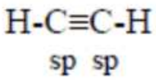
By using conventional formula it is not possible for the prediction of hybridization state of terminal carbon atom of alkynes as follows:

Ex.3. Hybridization state of Ethyne **(Fig. 2.12):**

By Conventional Formula: P = 1/2 (V+MA−C+A) = 1/2 (4+1-0) = 2.5 (Unpredictable hybridization state)

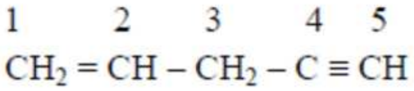
By Innovative Formula: (P_{Hyb}) = (T_{SLP}) – 1 = 2-1 = 1 (sp hybridized carbon atom in Alkyne)

where, P_{Hyb} = Power on the Hybridization state of the central atom, T_{SLP} = (Total no of σ bonds around each central atom + LP)



$$\underset{}{H}\text{-}\underset{sp}{C}\equiv\underset{sp}{C}\text{-}H$$

Figure 2.12: Linear structure of Ethyne(C_2H_2)



$$\overset{1}{CH_2} = \overset{2}{CH} - \overset{3}{CH_2} - \overset{4}{C} \equiv \overset{5}{CH}$$

Figure 2.13: Structure of pent-1-ene-4-yne

Ex.-4. Hybridization state of pent-1-ene-4-yne **(Fig. 2.13):**

By 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

(Unpredictable hybridization state C_5)

By Innovative Formula: (P_{Hyb}) for C_5 = (T_{SLP}) – 1 = 2-1 = 1 (sp hybridized C_5)

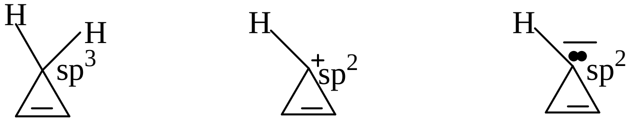
where, P_{Hyb} = Power on the Hybridization state of the central atom, T_{SLP} = (Total no of σ bonds around each central atom + LP)

By using conventional formula it is not possible for the prediction of hybridization state of oxygen atoms in cyclic ozone, hydrogen peroxide, S atom in S_8, P atom in P_4 etc. but by using innovative formula hybridization state in all cases should be determined with absolute accuracy.

B. A comparative study between conventional and innovative formula for prediction of hybridization state of carbon atom in different non-heterocyclic organic compounds

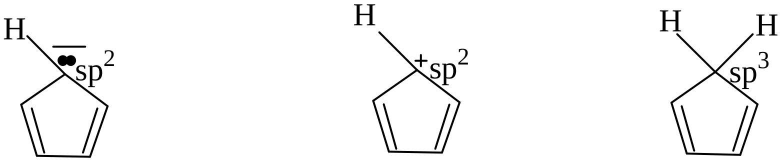
By using conventional formula it is not possible for the prediction of hybridization state of carbon atoms in cyclopropene, cyclopentadiene, cycloheptatriene, cyclopropenyl anion, cyclopentadienyl anion, cycloheptatrienyl anion, cyclopropenyl cation, cyclopentadienyl cation, and cycloheptatrienyl cation, benzene, toluene etc. but by using innovative formula hybridization state in all cases should be determined with absolute accuracy as follows:

By using conventional formulae hybridization state of vertex carbon atom in cycloalkenes such as cyclopropene, cyclopentadiene, cycloheptatriene etc. (**Fig. 2.14, Fig. 2.15, Fig. 2.16)** came out erroneous as follows:



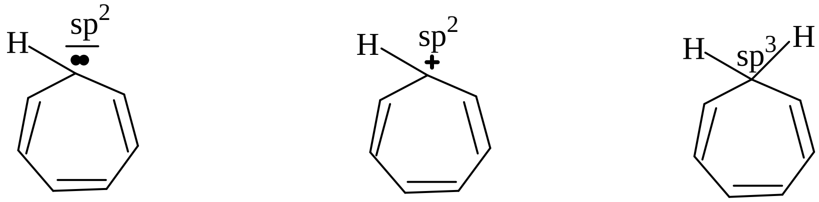
(Cyclopropene) (Cyclopropenyl cation) (Cyclopropenyl anion)

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

i)By using the conventional formula:

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)By using Innovative formula:

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

By using conventional formulae hybridization state of rest carbon atoms other than vertex carbon in cycloalkenes such as cyclopropene, cyclopentadiene and cycloheptatriene (**Fig. 2.14, Fig. 2.15, Fig. 2.16)** came out unpredictable as follows:

i)By using the conventional formula:

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) By using Innovative formula:

Power of the hybridization state, $(P_{Hyb}) = (T_{SLNC}) - 1 = 3-1 = 2$ (sp^2 hybridization state of rest carbons other than vertex carbon)

By using conventional formulae hybridization state of vertex carbon atom bearing negative charge in cycloalkenyl anions such as cyclopropenyl anion, cyclopentadienyl anion and cycloheptatrienyl anion (**Fig. 2.14, Fig. 2.15, Fig.2.16)** came out erroneous as follows:

i)By using the conventional formula:

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^2 - erroneous hybridization state)

ii) By using Innovative formula:

Power of the hybridization state of the vertex carbon, $(P_{Hyb}) = (T_{SLNC}) - 1 = 3-1 = 2$ (sp^2 hybridization state)

By using conventional formulae hybridization state of vertex carbon atom bearing positive charge in cycloalkenyl cation such as cyclopropenyl cation, cyclopentadienyl cation and cycloheptatrienyl cation (**Fig. 2.14, Fig. 2.15, Fig. 2.16)** came out erroneous as follows:

i)By using conventional formula:

Power of the hybridization state of the vertex carbon bearing positive charge, (P) = 1/2 (V+MA−C+A) = 1/2 {4+1-(1+0)}

= 1/2{4} =2 (sp - erroneous hybridization state)

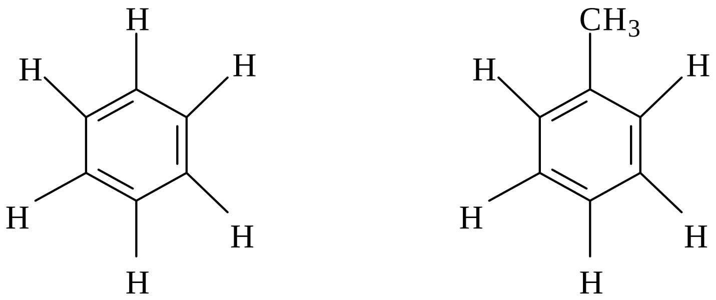
ii) By using Innovative formula:

Power of the hybridization state of the vertex carbon bearing positive charge, $(P_{Hyb}) = (T_{SLNC}) - 1 = 3-1$

$= 2$ (sp^2 hybridization state)

By using conventional formulae hybridization state of carbon atoms in benzene, toluene etc. is unpredictable but by using innovative formula hybridization state in all cases should be determined with absolute accuracy as follows:

The carbon atom in Benzene **(Fig.3.20):**



(Fig.3.20: Sructure of Benzene and Toluene)

i)By using the conventional formula:

Power of the hybridization state of carbon, (P) = 1/2 (V+MA−C+A) = 1/2 (4+1-0) = 2.5 (unpredictable hybridization state)

ii) By using Innovative formula:

Power of the hybridization state of carbon atom, $(P_{Hyb}) = (T_{SLNC}) – 1 = 3-1 = 2$ (sp^2 hybridization state)

Carbon atom of the methyl group in Toluene **(Fig.3.20):**

i)By using the conventional formula:

Power of the hybridization state of carbon atom of methyl group in toluene, (P) = 1/2 (V+MA−C+A) = 1/2 (4+3-0) = 3.5 (unpredictable hybridization state)

ii) By using Innovative formula:

Power of the hybridization state of carbon atom of methyl group in toluene, $(P_{Hyb}) = (T_{SLNC}) – 1 = 4-1 = 3$ (sp^3 hybridization state)

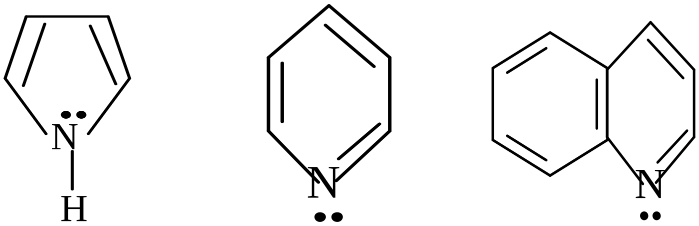
C. A comparative study between conventional and innovative formula for prediction of hybridization state of the heteroatom in different heterocyclic compounds

By using conventional formula it is not possible for the prediction of hybridization state of heteroatom nitrogen in pyridine, quinoline, isoquinoline, pyrimidine, thiazole, benzothiazole, pyrazine, cyanidine, phenazine, 1,2,3,4-tetrazine, azocine, azetine, aziridine, and oxygen atom in oxetan etc. but by using innovative formula hybridization state of heteroatom nitrogen in all cases should be determined with absolute accuracy as follows.

i)By using the conventional formula:

Power of the hybridization state of nitrogen atom in pyridine, $P = 1/2\ (V+MA-C+A) = 1/2\ (5 + 0 - 0 + 0) = 2.5$ **(Unpredictable hybridization state)** and power of the hybridization state of nitrogen atom in quinoline, $P = 1/2\ (V+H-C+A) = 1/2\ (5 + 0 - 0 + 0) = 2.5$ **(Unpredictable hybridization state) (Fig.2.18).**

Power of the hybridization state of nitrogen atom in aziridine, $P = 1/2\ (V+MA-C+A) = 1/2\ (5 + 1 - 0 + 0) = 3$ **(sp^2 – erroneous hybridization state of N)** and power of the hybridization state of oxygen atom in oxetan, $P = 1/2(V+MA-C+A) = 1/2\ (6 + 0 - 0 + 0) = 3$ **(sp^2 - erroneous hybridization state of oxygen atom) (Fig.2.19).**



Pyrrole Pyridine Quinoline

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

Aziridine Oxetan

Fig.2.19: Structure of aziridine and oxetan

ii) By using Innovative formula:

Power on the Hybridization state of the hetero atom $(P_{Hyb}) = (T_{SLLP}) - 1$

Power of the hybridization state of nitrogen atom in pyridine, $\mathbf{P_{Hyb}} = (3 - 1) = 2$ (σ bonds = 2 & LLP = 1) **(sp^2 hybridization state of N atom)** and power of the hybridization state of nitrogen atom in quinoline, $\mathbf{P_{Hyb}} = (3 - 1) = 2$ (σ bonds = 2 & LLP = 1) **(sp^2 hybridization state of N atom) (Fig.2.18).**

Power of the hybridization state of nitrogen atom in aziridine, $\mathbf{P_{Hyb}} = (4 - 1) = 3$ (σ bonds = 3 & LLP = 1) **(sp^3 hybridization state of N atom)** and power of the hybridization state of oxygen atom in oxetan, $\mathbf{P_{Hyb}} = (4 - 1) = 3$ (σ bonds = 2 & LLP = 2) **(sp^3 hybridization state of O atom) (Fig.2.19)**.

Conclusion

In this chapter, limitation of conventional formula and its comparative study have been discussed in the light of innovative formulae for the prediction of 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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