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

KEYWORDS: Central atom, Peripheral atom, sigma bond, Lone pair or e-s, Co-ordinate bond, UG and PG Level

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ABSTRACT *Prediction of hybridization state is a vitally important to students of chemistry in undergraduate, graduate and also in Post-graduate level. The method which is generally used for determination of hybridization state to find out the geometry is time consuming. To keep the matter in mind a new innovative method has to be introduced for calculation of hybridization state in a very simple way, which is also be a time savings one. Experiment in vitro on 100 number of students showed that for determination of Hybridization state, using old method,strike rate is 1Q/5min and by using these new innovative methods strike rate is 1Q/5secs. On the basis of this experiment I can strongly recommend that these new methods will be the very rapid one for the determination of hybridization state.*

INTRODUCTION

A clear understanding and prediction of hybridization states are vitally important to students of chemistry in undergraduate, graduate and also in Postgraduate level to solve different kind of problems related hybridization state[1,2,3]. The method which is generally used for determination of hybridization state is time consuming[4]. This new innovative method for prediction of hybridization states would go a long way to help to the students of chemistry who would choose the subject as their career.

We Know, Hybridization is nothing but the mixing of orbital's in different ratio to form some newly synthesized orbital's called hybrid orbitals. The mixing pattern is as follows:

Mixing		Hybrid orbital	Power of the Hybridization
s + p (1:1)	-	sp hybrid orbital	01
s + p (1:2)	-	sp^2 hybrid orbital	02
s + p (1:3)	-	sp^3 hybrid orbital	03

Formula for determination of hybridization state like sp, sp^2, sp^3 followed the following method:

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

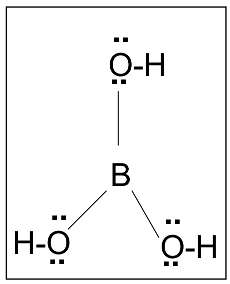
All single (-) bonds are σ bond, in double bond (=) there is one σ and 1π, in triple bond there is one σ and 2π. In addition to these each lone pair (i.e.no of electrons in the outermost orbit which should not take part in bond formation) and Co-ordinate bond can be treated as one σ bond.

Eg:-

1. In NH_3, centre atom N is surrounded by three N-H single bond i.e. three sigma (σ) bonds and one LP i.e. one additional σ bond. So, altogether in NH_3 there is four σ bonds (3BP + 1LP) around centre atom N, So, in this case Power of the Hybridization state of N = 4-1 =3 i.e. hybridization state=sp^3.

2. In H_2O, centre atom O is surrounded by two O-H single bond i.e. two sigma (σ) bonds and two LPs i.e. two additional σ bonds. So, altogether in H_2O there is four σ bonds (2BPs + 2LPs) around centre atom O, So, in this case Power of the Hybridization state of O = 4-1 =3 i.e. hybridization state of O in H_2O = sp^3.

3. In H_3BO_3 (AIEEE-04) -



B has 3σ bonds (3BPs but no LPs) and oxygen has 4σ bonds (2BPs & 2LPs)

so, in this case power of the hybridization state of B = 3-1 = 2 i.e. B is sp^2 hybridized in H_3BO_3. on the other hand, power of the hybridization state of O = 4-1= 3 i.e. hybridization state of O in H_3BO_3 is sp^3.

4. In I-Cl – I and Cl both have 4σ bonds (1BP and 3LPs), So, in this case power of the hybridization state of both I and Cl = 4-1= 3 i.e. hybridization state of I and Cl both are sp^3.

5. In CH_2=CH_2 – Each carbon is attached with 02 C-H single bonds (02 σ bonds) and one C=C bond (01σ bond), so, altogether there is 03 sigma bonds. So, in this case power of the hybridization state of both C = 3-1= 2 i.e. hybridization state of both C's are sp^2.

6. In N_2O (N≡N→O): The hybridization state of first N is sp due to one LP and one σ bond from N≡N and also the hybridization state of second N is sp due to one Co-ordinate bond and one σ bond from N≡N.

For determination of the hybridization state like sp^3d, sp^3d^2, sp^3d^3 followed the following method:-

In case of sp^3d, sp^3d^2 and sp^3d^3 hybridization state there is a common term sp^3 for which 04 sigma bonds are responsible. So, in addition to 04 sigma bonds, for each additional sigma, added one d orbital gradually as follows-

5σ bonds = 4σ bonds + 01 additional σ bond = sp^3d hrbridization.

6σ bonds = 4σ bonds + 02 additional σ bonds = sp^3d^2 hrbridization.

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7σ bonds = 4σ bonds + 03 additional σ bonds = sp^3d^3 hrbridization.

Eg:- 1.IF_7 - 7 I-F single bonds i.e. 7σ bonds = 4σ bonds + 03 additional σ bonds = sp^3d^3 hrbridization.

2. IF_4^+ - I has 07 e^-s in its outermost shell, so, in this case, subtract one e^- from 07 i.e. 07-1= 06. So, out of 06 electrons, 04 electrons form 04 I-F bonds i.e. 04 sigma bonds and there is one LP. So, altogether there is 05 σ bonds. So, 5σ bonds = 04 σ bonds + 01 additional σ bond = sp^3d hrbridization.

3. ICl_2^- - I has 07 e^-s in its outermost shell, so, in this case, add one e^- with 07 i.e. 07+1= 08.

So, out of 08 electrons, 02 electrons form 02 I-Cl bonds i.e. 02 sigma bonds and there is 03 LPs.

So,altogether there is 05σ bonds. So, 5σ bonds = 04 σ bonds + 01 additional σ bond = sp^3d hrbridization.

4. XeF_4- Xe, an inert gas, consider 8 e^-s in its outermost shell, 04 of which form 04 Xe-F sigma bonds and there is two LPs, i.e. altogether there is 06 σ bonds = 04 σ bonds + 02 additional σ bonds = sp^3d^2 hrbridization.

In case of determination of the hybridization state you must have a clear idea about the outermost electrons of different family members in the periodic table as follows:

Family	Outermost electrons
Nitrogen family	05
Oxygen family	06
Halogen family	07
Inert gas family	08

And in case of cationic species you must remove one electron from the outermost orbit of the central atom and incase of anionic species you must add one electron with the outermost electrons of the central atom.

CONCLUSIONS: This article is very helpful to students in chemistry of undergraduate,

graduate and also in Postgraduate level. This one be the very time savings method. By using this method student can predict hybridization state in a very simple way.

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