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The Concept of Hybridization : A Rapid and New Innovative Method for Prediction of Hybridized State of an Atom in a Very Short Time

KEYWORDS: Hybridization of Atomic Orbitals, Molecular Geometry, Electronic Structure, Undergraduate, Graduate, Postgraduate, Principle of Maximum Overlapping.

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ABSTRACT *For the prediction of molecular and electronic properties of a substance a clear understanding of the concept of hybridization is vitally important to students of chemistry in undergraduate, graduate and also in postgraduate level. Several studies have noted that the concept of hybridization is among one of the most difficult to understand for students at all levels of learning chemistry. There are various methods which are generally used to find the hybridized state of an atom and these methods are time consuming. In this work we discuss the concept of hybridization in detail and try to develop a physical picture of hybridization process. On the basis of our investigation of a large number of polyatomic molecules and ions, we report a new innovative method for prediction of hybridized state of an atom in a very short time without knowing the electronic structure of the molecule or ion. We can strongly recommend that this method will be the very rapid one for the determination of hybridized state of an atom.*

• INTRODUCTION

For the prediction of molecular and electronic properties of a substance a clear understanding of the concept of hybridization is vitally important to students of chemistry in undergraduate, graduate and also in postgraduate level.[1,2,3] Several studies have noted that the concept of hybridization is among one of the most difficult to understand for students at all levels of learning chemistry.[4] There are various methods which are generally used to find the hybridized state of an atom and these methods are time consuming.[5] Recently, Arijit Das[6] claimed a new innovative method for prediction of hybridized state in a very short time but when we go through the research article we found that the method was based on the electronic structure of the molecule. It is time consuming to first draw the electronic structure and then to calculate the number of σ-bonds, π-bonds, lone pairs etc. So, his method is also very much time consuming. On the basis of our investigation of a large number of polyatomic molecules and ions, we report a new innovative method for prediction of hybridized state of an atom in a very short time without knowing the electronic structure of the molecule or ion.

First we discuss the concept of hybridization in detail and try to develop a physical picture of hybridization process. Hybridization is a theoretical concept which was introduced by Linus Pauling.[7] The concept of hybridization is mainly used to predict the geometry of certain covalent bonded polyatomic molecules and ions. Hybridization is defined as the intermixing of dissimilar orbitals of the same atom but having slightly different energies to form same number of hybrid orbitals of equal energies and identical shapes.

• Significance or need of hybridization process

Using hybridization process we are able to explain the following observed facts :

(i) tetra valency of carbon, all C-H bond lengths are equal in CH_4 molecule as well all H-C-H bond angles are equal i.e. $109^0 28'$ (ii) geometry of certain covalent bonded molecules and ions (iii) existence and non-existence of certain molecules in nature (iv) relative bond strength of σ and π-bonds.

• Characteristics of hybridization process

(1) Hybridization takes place only in orbitals belonging to the same atom or ion.
(2) Orbitals of almost similar energies undergo hybridization. Hence a 2s orbital cannot be hybridized with 3s orbital as the energy difference is more. Both half filled or fully filled or vacant orbitals (in complexes) can involve in hybridization process.
(3) Generally, 'd' orbitals do not take part in hybridization process due to their very large size or high energy as compared to that of 's' and 'p' orbitals but mixing of 'd' orbitals takes place in the presence of more electronegative atom than the central atom due to contraction in the size of 'd' orbitals.
(4) After hybridization process we get the same number of hybridized orbitals as are participating in the mixing process according to the law of conservation of orbitals.
(5) All the hybridized orbitals obtained after mixing process have the same energy and shape but differ in their orientation.
(6) All the hybridized orbitals tend to be placed themselves as far apart from each other as possible to minimize the repulsive forces.
(7) Hybridized orbitals provide more efficient overlapping than overlapping by pure s, p and d-orbitals due to fixed orientation or more directional nature of hybridized orbitals. Hence, hybridization is also known as 'Principle of maximum overlapping'.[7,8]
(8) Hybridization never takes place in an isolated atom or ion but it occurs only when an atom or ion is undergoing to form covalent bonds with two or more atoms.

On the basis of above characteristics, we formulate the following facts for a clear understanding and prediction of hybridized state of an atom in a polyatomic molecule or ion.

(1) Generally, there is no hybridization process without involvement of s-orbital because s-orbital provides a base or platform for mixing of p and d orbitals.
(2) σ bonds are generally formed by axial overlapping of hybridized orbitals in a polyatomic molecule or ion.
(3) π-bonds are formed by lateral overlapping of pure p-orbitals or p and d-orbitals or d and d-orbitals of bonded atoms.
(4) Lone pairs on central atom of a molecule are generally considered to be present in hybridized orbitals provided if they are not involved in pπ-pπ, pπ-dπ bonding or in resonance.

• How to determine type of hybridization

In order to figure out the hybridized state of an atom, first we need to know the electronic structure of the molecule or ion then on the basis of electronic structure we can easily predict

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the hybridized state of concerned atom.

The structure of any molecule can be predicted on the basis of hybridization which in turn can be known by the following general formulation,

H = Nσ + LP

Where H= Number of orbitals involved in hybridization viz. 2, 3, 4, 5, 6 and 7, hence nature of hybridization will be sp, sp^2, sp^3, sp^3d, sp^3d^2, sp^3d^3 respectively.

Nσ = Number of σ bonds formed by concerned atom,

LP = number of lone pairs present on concerned atom excluding lone pair involved in pπ-pπ, pπ-dπ bonding or in resonance.

But the drawback of this formulation is that first we have to draw the electronic structure of the molecule which is time consuming process.

There is another formula which does not require the structure of the molecule or ion and is less time consuming,

H = ½ (V + M – C + A)

Where H = Number of orbitals involved in hybridization viz. 2, 3, 4, 5, 6 and 7, hence nature of hybridization will be sp, sp^2, sp^3, sp^3d, sp^3d^2, sp^3d^3 respectively.

V = Number of electrons in valence shell of the central atom,

M = Number of monovalent atoms

C = Charge on cation,

A = Charge on anion

This formula can not predict the hybridized state of that central atom which is bonded with multivalent atoms like P_4, P_2O_5, P_4O_{10} and so many other similar molecules and ions.

We formulate another method which can be applied for a large number of molecules and ions without knowing their structure and we are able to predict the hybridized state of an atom in a very short time.

H = ½ (V_e + M – C + A)

Where H = Number of orbitals involved in hybridization viz. 2, 3, 4, 5, 6 and 7, hence nature of hybridization will be sp, sp^2, sp^3, sp^3d, sp^3d^2, sp^3d^3 respectively.

V_e = Number of valence electrons of concerned atom,

M = Number of other atoms excluding concerned and C, O, S (carbon, oxygen and sulphur atoms)

C = Charge on cation,

A = Charge on anion

• Results and discussion of hybridized state of central atom of some molecules and ions

Now we take two examples and discuss the utility of our formulation to find the hybridized state of central atom in a very short time. According to the method reported by Arijit Das[6], to find hybridized state of N in ammonia molecule, first we have to draw the electronic structure and then we can find that in NH_3, central 'N' atom 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 are four σ bonds (3BP + 1LP) around central 'N' atom, So, in this case Power of the Hybridized state of N = 4-1 =3 i.e. hybridized state=sp^3. According to our formula i.e. H = ½ (V_e + M – C + A), for NH_3 molecule V_e=5, M=3, and H comes out 4 i.e. hybridized state=sp^3. Similarly, 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 are four σ bonds (2BPs + 2LPs) around central 'O' atom, So, in this case Power of the Hybridized state of O = 4-1 =3 i.e. hybridized state of O in H_2O = sp^3. Using our formula, H comes out 4 i.e. hybridized state of O in H_2O = sp^3 Results of predicted hybridized state of central atom using our method are given in Tables-1 to 7.

Table 1. Hybridized State of Beryllium, Boron and Carbon in Some Molecules and Ions.

S. No.	Formula of Molecule or Ion	(Ve)	M	C	A	H=½ (V_e+M-C+A)	Hybridized State of Central Atom
1.	BeF_2	2	2	-	-	2	sp
2.	$BeCl_2$	2	2	-	-	2	sp
3.	BF_3	3	3	-	-	3	sp^2
4.	BF_4^-	3	4	-	1	4	sp^3
5.	H_3BO_3	3	3	-	-	3	sp^2
6.	CH_4	4	4	-	-	4	sp^3
7.	CH_3^+	4	3	1	-	3	sp^2
8.	CH_3^-	4	3	-	1	4	sp^3
9.	CH_2	4	2	-	-	3	sp^2
10.	CCl_2	4	2	-	-	3	sp^2
11.	C_3O_2	4	0	-	-	2	sp
12.	CO_3^{2-}	4	0	-	2	3	sp^2
13.	$C_2O_4^{2-}$	4	0	-	2	3	sp^2

Table 2. Hybridized State of Nitrogen in Some Molecules and Ions.

S. No.	Formula of Molecule or Ion	(Ve)	M	C	A	H=½ (V_e+M-C+A)	Hybridized State of Central Atom
1.	NH_3	5	3	-	-	4	sp^3
2.	NH_4^+	5	4	1	-	4	sp^3
3.	NH_2^-	5	2	-	1	4	sp^3
4.	NO_2^+	5	0	1	-	2	sp
5.	NO_2^-	5	0	-	1	3	sp^2
6.	NO_3^-	5	0	-	1	3	sp^2
7.	HNO_2	5	1	-	-	3	sp^2
8.	HNO_3	5	1	-	-	3	sp^2
9.	N_2O_4	5	1	-	-	3	sp^2
10.	N_2O_5	5	1	-	-	3	sp^2
11.	NF_3	5	3	-	-	4	sp^3

Table 3. Hybridized State of Oxygen in Some Molecules and Ions.

S. No.	Formula of Molecule or Ion	(Ve)	M	C	A	H=½ (V_e+M-C+A)	Hybridized State of Central Atom
1.	H_2O	6	2	-	-	4	sp^3
2.	H_2O_2	6	2	-	-	4	sp^3
3.	H_3O^+	6	3	1	-	4	sp^3
4.	OF_2	6	2	-	-	4	sp^3
5.	O_3	6	0	-	-	3	sp^2

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Table 4. Hybridized State of Phosphorus in Some Molecules and Ions.

S. No.	Formula of Molecule or Ion	(Ve)	M	C	A	$H=\frac{1}{2}(V_e+M-C+A)$	Hybridized State of Central Atom
1.	PH_3	5	3	-	-	4	sp^3
2.	PCl_3	5	3	-	-	4	sp^3
3.	PCl_5	5	5	-	-	5	sp^3d
4.	$POCl_3$	5	3	-	-	4	sp^3
5.	H_3PO_2	5	3	-	-	4	sp^3
6.	H_3PO_3	5	3	-	-	4	sp^3
7.	H_3PO_4	5	3	-	-	4	sp^3
8.	P_4	5	3	-	-	4	sp^3
9.	P_2O_5	5	1	-	-	3	sp^2
10.	P_4O_{10}	5	3	-	-	4	sp^3
11.	PO_4^{3-}	5	0	-	3	4	sp^3

Table 5. Hybridized State of Sulphur in Some Molecules and Ions.

S. No.	Formula of Molecule or Ion	(Ve)	M	C	A	$H=\frac{1}{2}(V_e+M-C+A)$	Hybridized State of Central Atom
1.	SO_2	6	0	-	-	3	sp^2
2.	SO_3	6	0	-	-	3	sp^2
3.	SF_4	6	4	-	-	5	sp^3d
4.	SF_6	6	6	-	-	6	sp^3d^2
5.	H_2SO_3	6	2	-	-	4	sp^3
6.	H_2SO_4	6	2	-	-	4	sp^3
7.	H_2SO_5	6	2	-	-	4	sp^3
8.	$H_2S_2O_7$	6	2	-	-	4	sp^3
9.	$H_2S_2O_8$	6	2	-	-	4	sp^3
10.	$SOCl_2$	6	2	-	-	4	sp^3
11.	SO_4^{2-}	6	0	-	2	4	sp^3
12.	SO_3^{2-}	6	0	-	2	4	sp^3
13.	$S_2O_3^{2-}$	6	0	-	2	4	sp^3

Table 6. Hybridized State of Halogens in Some Molecules and Ions.

S. No.	Formula of Molecule or Ion	(Ve)	M	C	A	$H=\frac{1}{2}(V_e+M-C+A)$	Hybridized State of Central Atom
1.	$HClO_2$	7	1	-	-	4	sp^3
2.	$HClO_3$	7	1	-	-	4	sp^3
3.	$HClO_4$	7	1	-	-	4	sp^3
4.	ClO_2^-	7	0	-	1	4	sp^3
5.	ClO_2^+	7	0	1	-	3	sp^2
6.	ClF_3	7	3	-	-	5	sp^3d
7.	IF_3	7	3	-	-	5	sp^3d
8.	IF_5	7	5	-	-	6	sp^3d^2
9.	IF_7	7	7	-	-	7	sp^3d^3
10.	I_3^-	7	2	-	1	5	sp^3d

Table 7. Hybridized State of Xenon in Some Molecules.

S. No.	Formula of Molecule or Ion	(Ve)	M	C	A	$H=\frac{1}{2}(V_e+M-C+A)$	Hybridized State of Central Atom
1.	XeF_2	8	2	-	-	5	sp^3d
2.	XeF_4	8	4	-	-	6	sp^3d^2
3.	XeF_6	8	6	-	-	7	sp^3d^3
4.	$XeOF_2$	8	2	-	-	5	sp^3d
5.	$XeOF_4$	8	4	-	-	6	sp^3d^2
6.	XeO_3	8	0	-	-	4	sp^3

Limitation of our method is that this formula can not be used to predict hybridized state of an atom in compounds having cyclic rings or catenation.

• Conclusions

This article is very helpful to students in chemistry of undergraduate, graduate and also in postgraduate level. This one be the very time saving method. By using this method student can predict hybridized state of an atom in a very short time without knowing the electronic structure of the molecule or ion.

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