HYBRIDIZATION AND MOLECULAR GEOMETRY: A NUMBER GAME

Lokendra Kumar Ojha
Lovely Professional University, Punjab
Email: ojha.lokendra@gmail.com

ABSTRACT

Present article emphasize the new pedagogy to learn the hybridization and molecular geometry. It is always a challenge for the students to remember the hybridization and geometry of the molecule correctly. This topic has several importance in subjective and objective type questions and answers since in most of the competitive examination hybridization and molecular geometry always comprise a huge number of questions. Now in order to remember all the hybridization, this paper gives you a table of few numbers and those number are also no need to remember because they contain certain trends in period and column (subtract 8 in row and subtract 6 in column) and certainly the table will form. Here, the more focus on the domain number (total bond pair and lone pair) 6, 5 and 4 because these domain number contain various type of geometry. This article is not emphasizing the theory behind the hybridization, but only on how to remember different hybridization and their geometry as far as the competitive skill is concerned. It has also some of the restrictions (limitation) and may not work for some of the coordination complex and inorganic compounds. *[African Journal of Chemical Education—AJCE 7(1), January 2017]*

INTRODUCTION

Although the idea of orbital overlap allows us to understand the formation of covalent bonds, it is not always easy to extend these ideas to polyatomic molecules. When we apply valence-bond theory to polyatomic molecules, we must explain both the formation of electron-pair bonds and the observed geometries of the molecules.

The famous chemist Linus Pauling first developed the hybridization theory in 1931 in order to explain the structure of simple molecules such as methane (CH_4) using atomic orbitals [1]. Pauling explained this by supposing that in the presence of four hydrogen atoms, the s and p orbitals form four equivalent combinations or hybrid orbitals, each denoted by sp^3 to indicate its composition, which are directed along the four C-H bonds [2]. Hybridization happens when atomic orbitals mix to form new atomic orbitals. The new orbitals have the same total electron capacity as the old ones. The properties and energies of the new, hybridized orbitals are an 'average' of the original un-hybridized orbitals.

METHODOLOGY

In this methodology, only two numbers are taken into account and the rest of the numbers have certain trends in row and column. The row will start from number 48, and 6 is subtracted in row and 8 is subtracted in column.

For hybridization

In order to calculate the hybridization, we only need to sum the bond pair and lone pair. If the sum is equal to 2, then it is sp (one for s and one for p), and if it is equal to 3, then it is sp2 (one for s and two for p) and so on.

Table 1: For hybridization

Bond pair + Lone pair	Hybridization	Bond pair + Lone pair	Hybridization
2	**sp**	**5**	**sp^3d**
3	**sp^2**	**6**	**sp^3d^2**
4	**sp^3**	**7**	**sp^3d^3**

For e- pair geometry and hybridization

In order to find the e-pair geometry (molecular geometry), you only need to remember the numbers (total valence shell electron, TVE) given below. For example, any compound which has TVE equal to 40, it is always trigonal pyramidal and if it has TVE equal to 28, then it is T shaped and so on.

Table 2: For hybridization and e pair geometry

Domain 6			**Domain 5**			**Domain 4**		
TVE	**e- pair geometry**	**Hybridization**	**TVE**	**e- pair geometry**	**Hybridization**	**TVE**	**e- pair geometry**	**Hybridization**
48	Octahedral	**sp^3d^2**	**40**	Trigonal bipyramidal	**sp^3d**	**32**	Tetrahedral	**sp^3**
42	Square Pyramidal	**sp^3d^2**	**34**	See saw	**sp^3d**	**26**	Trigonal bipyramidal	**sp^3**
36	Square Planer	**sp^3d^2**	**28**	T shaped	**sp^3d**	**20**	Bent/ Angular/ V shaped	**sp^3**
			22	Linear	**sp^3d**			

Domain 4, 5 and 6 represent the coordination number of the central metal like if it is PCl_5, then the central metal atom (most electropositive metal, P) is connected with five chlorine atoms and it has 5 coordination number and so on.

In the table below (3), ML_nE stands for M = central metal atom, L= Ligand or most electronegative element, E= lone pair, n= 2, 3, 4, 5, 6 …). Coordination number 6 has three category of total valence electron i.e. 48, 42, 36 and all have sp^3d^2 hybridization, and similar phenomenon occurs for other coordination numbers. Here we avoid the use of sp and sp^2 hybridization because they have only single molecular geometry i.e. linear and trigonal.

CN 6	TVE	e- pair geometry	Molecular Geometry	CN5	e- pair geometry	TVE	Molecular Geometry	CN4	TVE	Molecular Geometry	e- pair geometry
ML_6	48	Octahedral	Octahedral	ML_5	Trigonal bipyramidal	40	Trigonal bipyramidal	ML_4	32	Tetrahedral	Tetrahedral
ML_5E	42	Octahedral	Square Pyramidal	ML_4E	Trigonal bipyramidal	34	See saw	ML_3E	26	Tetrahedral	Trigonal bipyramidal
ML_4E_2	36	Octahedral	Square Planer	ML_3E_2	Trigonal bipyramidal	28	T shaped	ML_2E_2	20	Tetrahedral	Bent/ Angular/ V shaped
				ML_2E_3	Trigonal bipyramidal	22	Linear				

RESULTS AND DISCUSSION

Now, in order to find out the hybridization and molecular geometry, you only need to remember the above table and it is nothing but subtraction of 8 in column and subtraction of 6 in row. First, we need to calculate all the valence shell electrons in given compound and then the compound must belong to one of the given above number.

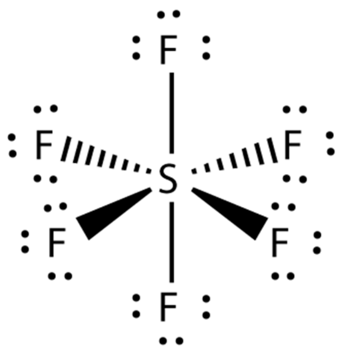
Let us, solve some of the examples:

Domain no 6

SF6 (Sulphur hexafluoride)

Total Valence Electron (TVE) = 6 + 7× 6= 48

Six bond pair (total 12 e-) connected with the six chlorine atoms and all six fluorine contain 36 lone pair electron (6 for each fluorine) i.e. it has no lone pair left in order to complete the total valence electron.



Total bond pair electron = 12

Total lone pair electron = 36 (6 for each six fluorine)

Total valence shell electron= 48

So, hybridization= total bond pair + total lone pair

6 + 0 = 5 i.e. **(sp^3d^2)**

Molecular (e^- pair geometry) = Octahedral (48)

Other examples PF_6, SiF_6^{2-}

$SbCl_5^{2-}$

Total Valence Electron (TVE) = 5 + 7× 5 +2= 42

Five bond pair (total 10 e-) connected with the five chlorine atom and all five chlorine contain 30 lone pair electron (6 for each chlorine) i.e. it has one lone pair left in order to complete the total valence electron.

Total bond pair electron = 10

Total lone pair electron = 30 (6 for each five chlorine)

Total valence shell electron= 40

So, hybridization= total bond pair + total lone pair

5 + 1 = 6 i.e. **(sp^3d^2)**

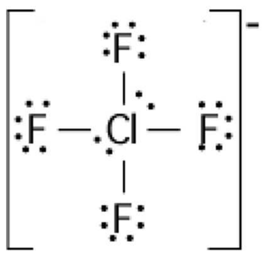
Molecular (e^- pair geometry) = Square Pyramidal (40)

Other examples PF_6, SiF_6^{2-}

ClF_4^-

Total Valence Electron (TVE) = 7 + 7× 4 +1= 36

Four bond pair (total 8 e-) connected with the four fluorine atom and all four fluorine contain 24 lone pair electron (6 for each fluorine) i.e. it has two lone pair left in order to complete the total valence electron.



Total bond pair electron = 8

Total lone pair electron = 28 (6 for each four fluorine and 4 for central chlorine atom)

Total valence shell electron= 36

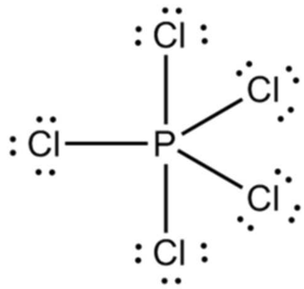
So, hybridization= total bond pair + total lone pair

4 + 2 = 6 i.e. **(sp^3d^2)**

Molecular (e^- pair geometry) = Square Planar (36)

Other examples ICl_4^-, XeF_4

PCl_5 (Phosphorus pentachloride)
Total Valence Electron (TVE) = 5 + 7× 5= 40
Five bond pair (total 10 e-) connected with the five chlorine atom and all five chlorine contain 30 lone pair electron (6 for each five chlorine) i.e. it has no lone pair left in order to complete the total valence electron.



Total bond pair electron = 10

Total lone pair electron = 30 (6 for each five chlorine)

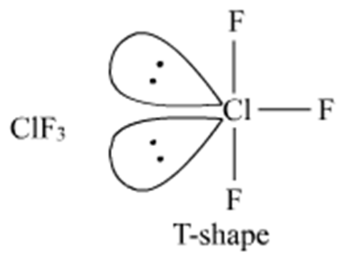
Total valence shell electron= 40

So, hybridization= total bond pair + total lone pair

5 + 0 = 5 i.e. **(sp^3d)**

Molecular geometry= Trigonal bipyramidal (40)

ClF_3 (Chlorine trifluoride)
Total Valence Electron (TVE) = 7 + 7× 3= 28
Three bond pair (total 6 e-) connected with the fluorine atom and all three fluorine contain 18 lone pair electron (6 for each fluorine) i.e. it has two lone pair left in order to complete the total valence electron.



Total bond pair electron = 6

Total lone pair electron = 22 (18 at three fluorine and 4 at chlorine)

Total valence shell electron= 28

So, hybridization= total bond pair + total lone pair

3 + 2 = 5 i.e. **(sp^3d)**

Molecular geometry= T shaped (28)

IF_4^+
Total Valence Electron (TVE) = 7 + 7× 4 - 1= 34
Four bond pair (total 8 e-) connected with the fluorine atom and all four fluorine contain 24 lone pair electron (6 for each fluorine) i.e. it has one lone pair left in order to complete the total valence electron.

Total bond pair electron = 8

Total lone pair electron = 26 (22 at four fluorine and 2 at chlorine)

Total valence shell electron= 34

So, hybridization= total bond pair + total lone pair

4 + 1 = 5 i.e. **(sp^3d)**

Molecular geometry= See Saw (34)

Other examples are ICl_3, TCl_4, PCl_5

I_3^-

Total Valence Electron (TVE) = 7× 3 +1= 22

Two bond pair (total 4 e-) connected with the iodine atom and all two iodine contain 12 lone pair electron (6 for each iodine) i.e. it has six lone pair left in order to complete the total valence electron.

Total bond pair electron = 4

Total lone pair electron = 18(12 at two corner iodine and 6 at central iodine atom)

Total valence shell electron= 22

So, hybridization= total bond pair + total lone pair

2 + 3 = 5 i.e. **(sp^3d)**

I_3^-

Molecular geometry= Linear (22)

Other examples XeF_2, ICl_2^-

Limitation

1. It has no explanation about the inner and outer d block configuration. No difference create between d^2sp^3 and sp^3d^2 because it is part of coordination compound where it can be explain accurately.
2. In coordination number four, there are three category (32. 26, 20) but if the TVE is equal to 8 then it is also consider in this domain and then you need to remember the general formula for particular domain.

Domain no 2

NH_3 (Ammonia)

Total Valence Electron (TVE) = 5 + 1× 3= 8

Three bond pair (total 6 e-) connected with the three hydrogen atom and it has one lone pair left in order to complete the total valence electron.

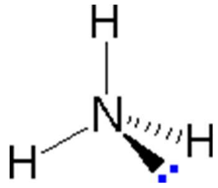
Total bond pair electron = 6

Total lone pair electron = 2 (for nitrogen atom)

Total valence shell electron= 8

So, hybridization= total bond pair + total lone pair

3 + 1 = 4 i.e. **(sp^3)**



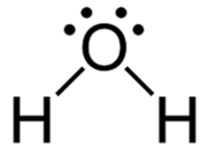
As it has three bond pair and one lone pair then it comes under the category of ML_3E

Molecular (e^- pair geometry) = Trigonal pyramidal (8)

Other examples H_3O^+

H_2O (Water)
Total Valence Electron (TVE) = 6 + 1× 2= 8
Two bond pair (total 4 e-) connected with the two hydrogen atom and it has two lone pair left in order to complete the total valence electron.

Total bond pair electron = 4



Total lone pair electron = 4 (for oxygen atom)

Total valence shell electron= 8

So, hybridization= total bond pair + total lone pair

2 + 2 = 4 i.e. **(sp^3)**

As it has three bond pair and one lone pair then it comes under the category of ML_2E_2

Molecular (e^- pair geometry) = Bent/ Angular/V shaped (8)

CONCLUSION

Problems (especially multiple-choice questions) can be solved easily, fast and accurately by using this technique. It has great importance in inorganic chemistry, especially coordination chemistry. Most of the problem is solved by using this method and it has some restrictions in CN 4 category of compounds.

REFERENCES

1. Pauling, L. (1931), "The nature of the chemical bond. Application of results obtained from the quantum mechanics and from a theory of paramagnetic susceptibility to the structure of molecules", Journal of the American Chemical Society, 53 (4): 1367–1400
2. Pauling, L. (1960). The Nature of the Chemical Bond (3rd ed., Oxford University Press) p.111–120.