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Research Paper

Straightforward Numerical Method to Understanding the Valence Shell Electron Pair Theory (VSEPR)

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ABSTRACT

It is well-known that Valence shell pair repulsion (VSEPR) hypothesis is customarily typically used to correctly predict molecular geometry. Be that as it may, it is firm to investigate the broad implications of this hypothesis by essentially drawing the molecular structure. This numerical procedure is constitutional and straightforward. This effective strategy can be actualized in science training at both the secondary school and college levels. This paper talked about the few examples of a straightforward molecular structure forecast. Properly utilizing the numerical procedure, both molecular geometry and the logical support can be imagined effortlessly.

Keywords: Bond pairs, Lone pairs, VSEPR theory

INTRODUCTION

The interpretation of structure and chemical reactions in Chemistry is usually supported semi-quantitative methodology during this paper used mathematical illustrations of electrons in a molecule and strategies for predicting their shapes. One of a more clearly properties of a material is its shape. Clearly, it is very significant to know the shape of a molecule for understanding its reactions. Practical applications of the prevalent VSEPR effective method reasonably require some simplifying assumptions about the unique nature of the bonding. Some valuable information is also needed before one can follow successfully the specific VSEPR rules. Molecular geometries can be satisfactorily explained implementing Lewis structures, VSEPR theory, Valence bond theory, Hybridization theory, and Molecular orbital theory, at this place we primarily use VSEPR theory. [2] To accurately determine molecular geometry, it is important to properly understand the essential difference between bonding electron pairs and non-bonding electron pairs. Bonding pairs are electrons shared by the central atom and other atoms, while non-bonding pairs are electrons on an individual atom that are unshared with another atoms. The term electron pair geometry typically refers to the bonding and non-bonding electron pair, molecular geometry accurately describes the resulting bond angles between the central and terminal atoms, which together predict the shape of a molecule. The molecular geometry can be predicted using the VSEPR theory. Electron pairs or group of electron pairs in the valence shell of an atom are known as the electron pair. [1] A bonding pair (BP) contains the electrons are shared between two same or different atoms as a single, double and triple bond, while a non-bonding pair or lone pair (LP) contains valence electrons in a central atom. It is the

straightforward numerical method to predict the geometries of compounds. It is simple and easy to understanding and properly using this method students can accurately predict the molecular shape and properly understand the moral justification according to VSEPR theory.

Table 1: valence electrons (VE) present in the outer most shell of the main group elements. [2]

VE / Period	1	2	3	4	5	6	7	8
2nd	Li	Be	B	C	N	O	F	Ne
3rd	Na	Mg	Al	Si	P	S	Cl	Ar
4th	K	Ca	Ga	Ge	As	Se	Br	Kr
5th	Rb	Sr	In	Sn	Sb	Te	I	Xe
6th	Cs	Ba	Tl	Pb	Bi	Po	At	Rn
7th	Fr	Ra						

THEORETICAL METHOD

The elements are listed in the periodic table in order of atomic number, not atomic weight because the atomic number tells us the number of valence electrons present in the outermost shell of the atom and it is very useful quantity to understanding VSPER theory. The horizontal rows are periods and vertical columns are groups, the numbering systems in the group's follows IUPAC rule. The periodic table is divided into s, p, d and f block, the s and p blocks collectively called as main group elements as shown as table 1. (Not shown H & He).

The proper shape of a molecule is depending on total number of valence electrons presents in a molecule. It has been identified adjustments are made by considering the differences in electrostatic repulsion between bonding pairs and lone pairs, the order are assuming to be in following sequence. [2]

LP-LP > LP-BP > BP -BP

The following rule is the properly use for understanding geometry of a molecule.

Table 2: Divisible Factor to total number of valence electrons.

Rule	Total number of valence electrons of a molecule	Factor
1	Less than8 (< 8)	Divide by factor 2
2	Greater than 8 (>8)	Divide by factor 8
3	Greater than 68 (> 68)	Divide by factor 18

Table 3. The description of molecular shape. [2,3] (BP- Bonding pair and LP- Lone pair)

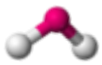
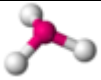
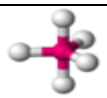
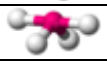
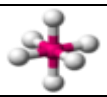
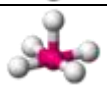
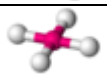
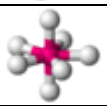
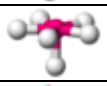
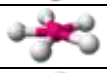
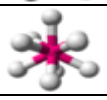
Factor	Hybridisation	BP	LP	Formula	Geometry	Shape	Bond Angle	Example
1	-	1	0	MX	Linear	M-X	-	BrCl, ClF
2	Sp	2	0	MX_2	Linear		180^0	$BeCl_2$,
3	Sp^2	3	0	MX_3	Trigonal Planer		120^0	BF_3, SO_3
		2	1	MX_2L	Bent or Angular		120^0	SO_2
		4	0	MX_4	Tetrahedral		109^0 28'	CH_4, $S0_4^{2-}$, NH_4^+
4	Sp^3	3	1	MX_3L	Pyramidal		$<109^0$ 28'	NH_3, SO_3^{2-}
		2	2	MX_2L_2	Bent or Angular		$< 109^0$ 28'	H_2O, O_3, NO_2^{2-}
		5	0	MX_5	Trigonal bi-pyramidal		120^0& 90^0	PCl_5 ,
5	Sp^3d	4	1	MX_4L	See Saw		90^0,120^0, &180^0	SF_4
		3	2	MX_3L_2	T-Shape		90^0&120^0	ClF_3, PF_3
		2	3	MX_2L_3	Linear		180^0	XeF_2

Table 3 to be continued…

		6	0	MX_6	Octahedral		90^0	SF_6
6	Sp^3d^2	5	1	MX_5L_1	Square pyramidal		90^0	ClF_5
		4	2	MX_4L_2	Square planer		90^0	XeF_4
		7	0	MX_7	Pentagonal bi-pyramidal		90^0, 72^0, 180^0	IF_7
7	Sp^3d^3	6	1	MX_6E	Pentagonal pyramidal		72^0, 90^0, 144^0	$XeOF_5^-$
		5	2	MX_5E_2	Planer pentagonal		72^0, 144^0	XeF_5^-
8	Sp^3d^4	8	0	MX_8	Square antiprismatic		60^0, 90^0	XeF_8^{2-}
9	Sp^3d^5	9	0	MX_9	Tricapped trigonal prismatic		--	ReH_9^{2-}

RESULTS AND DISCUSSION

Examples:

1. H_2O molecule:

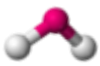
Total number of valence electrons = O + 2H
= 6 + 2
= 8

	Total number of valence electrons	Factor
2	08	4
	- 08	
	00	

Contributing Factor: 4, it means precisely it shows sp^3 hybridisation see the table 2, the molecule has two BP and two LP on the central atom.

Factor	BP	LP	Geometry
4	2	2	Bent

H_2O



2. PF_3 molecule:

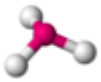
Total number of valence electrons = P + 3F
= 5 + 3x7
= 26

	Total number of valence electrons	Factor
8	26	3
	- 24	
2	02	1
	- 02	
	00	

Contributing Factor: 3 + 1 = 4, it shows sp^3 hybridisation, see the table 2, the molecule has three BP and one LP on the central atom.

Factor	BP	LP	Geometry
4	3	1	Pyramidal

PF_3



3. PCl_6^- molecule:

Total number of valence electrons
= P + 6Cl + 1 (- ve charge)
= 5 + (6 x 7) + 1
= 48

	Total number of valence electrons	Factor
8	48	6
	- 48	
	00	

Contributing Factor: 6, it shows sp^3d^2 hybridisation, see the table 2, the molecule has six BP and Zero LP on the central atom.

Factor	BP	LP	Geometry
6	6	0	Octahedral

PF_6

4. XeF_8^{2-} molecule:

Total number of valence electrons
= Xe + 8F + 2 (-ve charge)
= 8 + (8 x 7) + 2
= 66

	Total number of valence electrons	Factor
8	66	8
	- 64	
2	02	1
	- 02	
	00	

Contributing Factor: 8 + 1 = 9, it shows sp^3d^5, see the table 2.

XeF_8^{2-}

Tricapped trigonal prismatic

5. NH_4^+ molecule:

Total number of valence electrons

= N + 4H – 1 (+ve charge)

= 5 + (4 x 1) – 1

= 8

	Total number of valence electrons	Factor
2	08	4
	- 08	
	00	

Contributing Factor: 4, it shows sp^3 hybridisation, see the table 2.

The molecule has tetrahedral geometry.

NH_4^+

It is easy to calculate the factor if the negative charge on a molecule addition of the same number of electrons and the positive charge on a molecule subtract the same number of electrons from total number of valence electrons. In this method if remainder one it is added in a factor value.

CONCLUSION

The numerical methodology is straightforward, helpful and complex in understanding VSEPR theory as compared to alternative strategies, high school and undergraduate students will accurately predict the molecular shapes and understanding the justification consistent with VSEPR theory.

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