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A complement of valence shell electron pair repulsion (VSEPR) theory

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ABSTRACT

VSEPR model is extremely powerful in predicting the shapes of molecules and ions. Yet many students continue to experience some difficulty in utilizing it. This article has advanced a simple equation LP = ½ (g-b-c) which is readily applicable to mononuclear molecules or ions to determine the number of electron pairs around the central atom. Knowing the number of lone pairs, the geometry of the molecule or ion is easily deduced.

Key words: VSEPR theory, electron pairs, geometry.

INTRODUCTION

Every undergraduate student encounters the versatile VSEPR theory in chemistry subjects[1-5].

The theory which was advanced by renowned scientists Ronald Gillespie and Ronald Nyholm[6-11] is exceedingly useful in predicting the shapes of many mononuclear molecules and ions. If 'A' is taken as a central atom and 'B' as a 'ligand', then a general formula of the mononuclear species can be presented as AB_n (where n = 1, 2, 3, 4, 5, 6, ….). In this case B can be an atom or a pair of electrons. According to the VSEPR theory, the ideal shapes of common geometries of AB_n for n =1 to 6 are shown in Fig.1 below.

Since B could represent a pair of electrons (E), then we can have other possible derivative geometries.

AB→A-B linear; AB_2→B-A-B linear ;

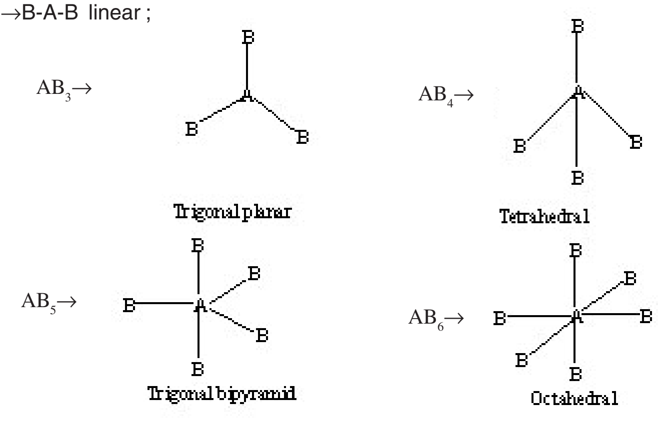


Fig. 1: Ideal geometries of ABn (n = 1 -6)

These include for $AB_3 \rightarrow AB_2E$; $AB_4 \rightarrow AB_3E$, AB_2E_2; $AB_5 \rightarrow AB_4E$, AB_3E_2, and AB_2E_3; $AB_6 \rightarrow AB_5E$, AB_4E_2.

In general, the molecular or ionic species with one or more electrons pairs E, will adopt the ideal geometry of the corresponding species which have no lone pairs except that in this case one or more of the atomic sites will be occupied by the electron pair(s).

Determining the Presence of Electron Pairs (E) in a Chemical Formula

Many undergraduate students experience some difficulty in determining whether or not the central atom has a lone pair or more. This creates some difficulty in predicting the ideal geometry of a given formula of a molecule or ion.

It is possible to easily determine the number of electron pairs on the central atom and hence the 'ideal' geometry for given formula AB_n where A and B are from Main Group Elements. I hereby present the simple equation that is versatile and extremely useful in determining the number of electron pairs around a given central atom.

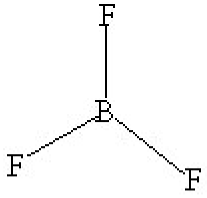
$LP = \frac{1}{2}(g-b-c)$, LP = Number of lone pairs, g = group number of the central atom, b = number of bonds linking up the ligands to the central atom, c = charge on the chemical species

Applications of the equation

Let us select some examples to illustrate the applications of the equation.

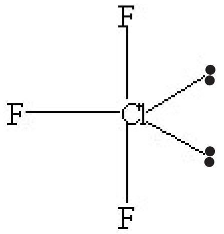
BF_3

B is in group three. Hence g = 3, F is monovalent and hence the number of bonds from the central atom linking up the ligands will be three. Hence b = 3. BF_3 is a neutral molecule and hence c = 0. Therefore the number of electron pairs on B will be given by $LP = \frac{1}{2}(3-3-0) = 0$. Thus, BF_3 will have a trigonal planar geometry with no lone pair of electrons.



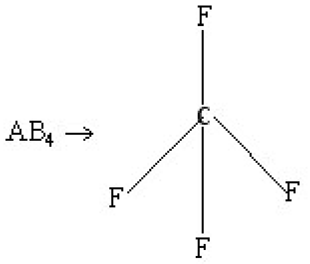
ClF_3

ClF_3 has a similar molecular formula as BF_3. However for ClF_3, g =7, b = 3, c =0. Hence, $LP = \frac{1}{2}(7-3-0) = 2$. Hence the geometry will be a trigonal bipyramid derivative (T-shape) of the form AB_3E_2.



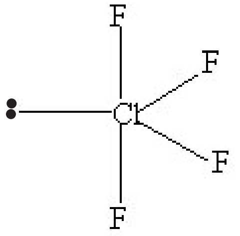
CF_4

The VSEPR variables for ClF_4 will be g =4, b=4, c =0. Hence LP = 0. This geometry is simply AB_4 type. That is tetrahedral.

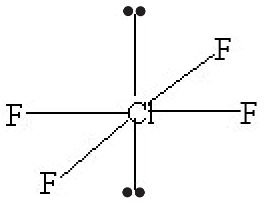


ClF_4^+

The VSEPR variables are g =7, b=4, c = 1. Hence $LP = \frac{1}{2}[7-4-(1)]=1$. Hence ClF_4^+ has one lone pair. The ionic species belongs to AB_4E type(distorted tetrahedral; a trigonal bipyramid derivative).

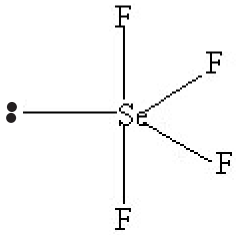


Following the same approach, g = 7, b=4, c = -1. Hence, g= ½ [7-4-(-1)] = 2. This means there are 2 lone pairs of electrons on Cl. The ionic species belongs to AB_4E_2 type (Square planar; octahedral derivative).



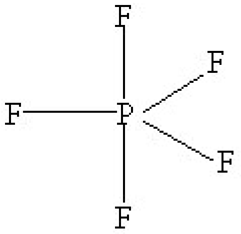
SeF_4

In this example, g=6, b=4, c =0. Therefore LP = ½ (6-4-0) =1. This means SeF_4 belongs to AB_4E type(distorted tetrahedral; trigonal bipyramid derivative).



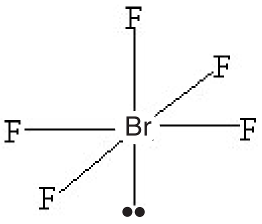
PF_5

Applying the equation we get, LP = ½ (5-5-0) = 0. This belongs to AB_5 type (trigonal bipyramid).



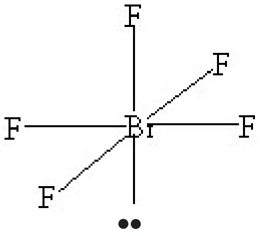
BrF_5

The number of lone pairs on Br will be given by LP = ½ (7-5-0) =1. The molecule belongs to AB_5E type (square pyramid; octahedral derivative).



SF_5^-

For SF_5^- , LP = ½[6-5-(-1)]=1. The ion belongs to AB_5E type (square pyramid; octahedral derivative).



The oxo compounds

The equation can also be adapted to other chemical species such as the oxo compounds. Examples

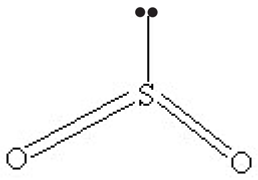
CO_2

In this case, the oxygen atom is taken as divalent. There are two bonds linking it to the C atom. Hence b=2 for each of the oxygen atom. Hence LP = ½ (4-4-0) = 0. This means there is no lone pair on carbon atom. Hence, the geometry will be linear. It may be regarded to belong to AB_2 type.

O=C=O

SO_2

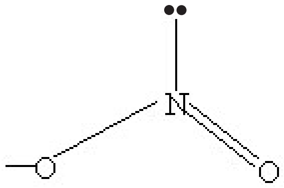
LP = ½ (6-4-0) = 1. Hence SO_2 may be considered to belong to AB_2E type(V-shape; trigonal planar derivative).



NO_2^-

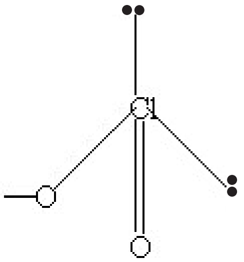
LP = ½ [5-4-(-1)] =1. Hence NO_2^- has a lone pair on the N atom.

The geometry will be as in SO_2 except that it is better to put the negative charge on one of the oxygen atoms.



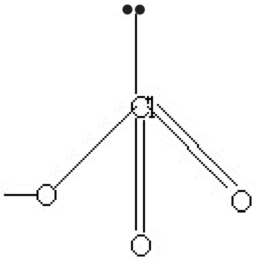
ClO_2^-

LP = ½[7-4-(-1)]= 2. This indicates that ClO_2^- has 2 lone pairs on Cl. The ion belongs to AB_2E_2 type (V-shape, tetrahedral derivative).



ClO_3^-

LP = ½ [7-6-(-1)] =1. The ClO_3^- ion has 1 lone pair. Hence, it belongs to AB_3E type (triangular pyramid; tetrahedral derivative).



CONCLUSION

This article presents a simple equation for determining whether or not a central atom in a mononuclear chemical species from the main group elements possesses a lone pair (lone pairs)of electrons. The equation is given by LP= ½(g-b-c).

Where LP-is the number of lone pairs, g-is the group of the central atom, b-is the number of bonds linking the central atom to the 'ligands' and c-is the charge on the chemical species.

REFERENCES

1. Changs, R, " *Chemistry,*" 3rd Edition, Random House, New York, 346 (1987).
2. Mortimer, C. E., "*Chemistry*, A Conceptual Approach", D. Van Nostrand Company, New York, 110 (1979).
3. Shriver, D. F., Atkins, P. W., "*Inorganic Chemistry*", 3rd Edition, Oxford Press, 74(1999).
4. Winter, M. J.,"*Chemical Bonding*", Oxford Science Publications, Oxford, 57 (1994).
5. Brady, J. E., Humiston, G. E., "*General Chemistry, Principles and Structure*", John Wiley and Sons, New York, 182 (1986).
6. Bader, F. W., Gillespie, R. J., MacDaougall, *J. Am, Chem., Soc.*, **110**: 7329 (1988).
7. Gillespie, R. J., and Nyholm, R. S., *Quart. Rev.*, **11**: 339(1957).
8. Gillespie, R. J., *J. Chem. Educ.*, **47**: 18(1970).
9. Gillespie, R. J., Robinson, E. A., *Chem. Soc. Rev.*, **34**: 396 (2005).
10. Gillespie, R. J., *Can. J. Chem.*, **70**: 742 (1992).
11. Gillespie, R. J., " *Molecular Geometry*", Van Nostrand Reinhold, London, (1972).