Turkish Journal of Computer and Mathematics Education Vol.12 No. 11 (2021), 3804- 3806
Research Article

Group Theory In Molecular Symmetry

[1]Jita Dutta, [2]Mukul Buragohain
[1]Assistant Professor, Department of Mathematics, Kakojan College, Jorhat, Assam
[2]Assistant Professor, Department of Mathematics, Digboi College, Digboi, Assam

Article History: Received: 11 January 2021; Revised: 12 February 2021; Accepted: 27 March 2021; Published online: 10 May 2021

ABSTRACT: Symmetry is one of the most pervasive concepts in the universe. It is used in our everyday language in two meanings. In the one sense symmetry means something like well-proportioned, well-balanced and the other sense. Symmetry denotes the sort of concordance of several parts by which they integrate into a whole. The study of symmetry provides one of the most appealing applications of group theory. The systematic mathematical treatment of symmetry is called group theory. Group theory is a rich and powerful subject by which we shall confine our use of it at this stage classification of molecules in terms of their symmetry properties, the construction of molecular orbitals and the analysis of molecular vibrations. To make the idea of molecular symmetry as useful as possible we must develop some rigid mathematical criteria of symmetry. Group theory is the tool by means of which generalizations concerning molecular symmetry are applied. In the advanced study of inorganic chemistry a systematic study of symmetry and the ways of specifying it with mathematical precision are important because wide variety of symmetric structure encounted.

Keywords: Symmetry operations, symmetry elements, molecular symmetry, schonflies system, symmetry groups

INTRODUCTION

Symmetry governs the physical and spectroscopic properties of molecules. Sets of symmetry operations constitute a mathematical group. Group theory is the mathematical application of symmetry to an object to obtain knowledge of its physical properties. By using the properties of groups, we can take advantage of molecular symmetry in a systematic way to predict the properties of molecules and to simplify molecular calculations. Molecular symmetry is a fundamental concept in Chemistry. The simple intuitive grasp of symmetry that most observant people naturally acquire is adequate for understanding chemistry up to a point. Many molecules have a certain degree of symmetry; methane is a tetrahedral molecule; benzene is hexagonal and so on. But in order to make the idea of molecular symmetry as useful as possible we must develop some rigid mathematical criteria of symmetry. We shall consider the kinds of symmetry elements that a molecule may have and the symmetry operations generated by the symmetry elements. We shall use the general properties of groups to aid in correctly and systematically determining the symmetry operation of any molecule [3].

SYMMETRY ELEMENTS AND OPERATIONS

A symmetry element is a geometrical entity such as a line, a plane or a point with respect to which one or more symmetry operations may be carried out. On the other hand a symmetry operation is a movement of a body such that, after the movement has been carried out, every point of the body is coincident with an equivalent point of the body it is original orientation [3].
There are two systems of symbols for representing symmetry elements:
(i) The Schonflies system, which is used primarily for molecular geometry and group theory.
(ii) The Hermann-Mauguin system, which is used in crystallography.
In this paper the researcher will adopt the conventional use of the Schonflies symmetry notation. For single molecules there are five symmetry elements and corresponding symmetry operations.

Table – 1

Symmetry Operation	Symmetry Element	Symbol
1. Identity	Whole of space	E
2. Rotation by $360^0/n$	n – fold symmetry axis	C_n
3. Reflection	Mirror plane	□
4. Inversion	Centre of inversion or centre of symmetry	i
5. Rotation by $360^0/n$ followed by reflection in a plane perpendicular to the rotation axis	n-fold axis of improper rotation	S_n

1. Identity E:
The identity operation consists of doing nothing to the molecule. All molecules and other finite bodies – possess identity symmetry. The E-operation although apparently trivial is involved in group theoretical calculations.

2. n-fold axis of symmetry (rotation axis):
A rotation operation C_n (n=1,2,3…) moves a body from a given orientation to an indistinguishable orientation for a rotation of $\frac{2\pi}{n}$ about the C_n axis. The water molecule possesses one twofold axis of symmetry (C_2). The highest fold rotation axis of a molecule is conventionally taken as the vertical z-axis.

3. Reflection (Mirror Plane) □:
A reflection symmetry plane □ relates the halves of a molecule, across that plane, as an objective is related to its mirror image. If the reflection plane contains the principle axis it is called vertical □**v;** if it is normal to the plane principle axis it is called horizontal □**h**. Diagonal planes □**d** are vertical planes that bisect the angles between successive two fold axes [7]
The water molecule possesses tow planes of symmetry. The plane in which the three atoms lie and the plane perpendicular to that plane and bisecting the H-O-H angle. Since the planes are 'vertical' in the sense of containing the rotational axis of the molecule they are laballed □v and □′**v**.

4. Inversion (Centre of Symmetry) i:
The inversion operation i through a point corresponding to a centre of symmetry and involves taking each part of the molecule, in a straight line, through the point to an equal distance on the other side. In an octahedral molecule (AB_6) with the point at the centre of the molecule, diametrically opposite pairs of atoms at the corners of the octahedron are interchanged.

5. n-fold rotation – reflection axis (improper rotational axis), s_n:
An improper rotation is thought as a combination of a proper rotation and a reflection through a plane perpendicular to the axis of rotation. The axis about which this occur is called an improper axis and is denoted by S_n, where n is the order of the axis. The operation of improper rotation by $\frac{2\pi}{n}$ is also denoted by the symbol s_n. It is seen that

S_5 = C_5 (then σ Reflection)
S_5^2 = C_5^2
S_5^3 = C_5^3 then □
S_5^4 = C_5^4
S_5^5 = □
S_5^6 = C_5
S_5^7 = C_5^2 then □
S_5^8 = C_5^3
S_5^9 = C_5^4 then □
S_5^{10} = E

In general the element S_n with n odd generates 2n operation [3]
Let us consider a four-fold improper rotation of a CH_4 molecule. In this case, the operation consists of a 90^0 rotation about an axis bisecting two HCH bond angles followed by a reflection through a plane perpendicular to the rotation axis.
Again we consider the two fold axes c_2 (x) and c_2 (y) coincide with the co-ordinate axes. Then we have –

$[x_1, y_1, z_1]\ c_{2\,(x)} \rightarrow [x_1, -y_1, -z_1]\ c_{2\,(y)} \rightarrow [-x_1, -y_1, z_1]$
i.e. $c_2(y)\, c_2(x) = c_2(z)$
i.e. whenever c_2 (x), c_2 (y) exist then c_2 (z) also exists.
Again □ (xz) is reflection through xz plane is □ (xz) $[x_1, y_1, z_1] \rightarrow [x_1, -y_1, z_1]$
Also $c_4(z)\ [x_1, y_1, z_1] \rightarrow [y_1, -x_1, z_1]$
Which gives c_4 (z) □ (xz) $[x_1, y_1, z_1] \rightarrow c_4(z)\ [x_1, -y_1, z_1] \rightarrow [-y_1, -x_1, z_1]$
i.e. □d $[x_1, y_1, z_1] \rightarrow [-y_1, -x_1, z_1]$
In this way we can calculate the effect of other elements. [3].

SYMMETRY GROUPS
A complete set of symmetry operation for a particular molecule is the set of operations in which every possible product of two operations is in the set. This set will form a group because it satisfies all the four criteria of a Mathematical group. These groups are known as Symmetry groups.
The Symmetry groups may be systematically classified by considering how to build them up using increasingly more elaborate combinations of Symmetry operations.

GROUPS WITH LOW SYMMETRY
There are three groups of low Symmetry that posses only one or two Symmetry elements.

(a) C_1 – If a molecule has only the identity element (E) that the groups is of order 1 and is called C_1 – group. For example CHBrClF molecule.
(b) C_s – In addition to the symmetry element E, which all molecules posses, these molecules contain a plane of symmetry. Examples of C_s symmetry are thionyl halides and Sulfoxides and Secondary amines.
(c) C_i – If a molecule has two symmetry operations only on the plane then they are □, □^{2} = E. This group is denoted by C_2. But we see that in a molecule whose sole Symmetry is an inversion centre then they are i, i^2 = E. Hence, a group of order 2 is denoted by C_i. For example : R, S -1, 2 – dichloro – 1, 2 – difluoroethane.

GROUPS WITH VERY HIGH SYMMETRY

These Symmetry groups may be defined by the large number of characteristic symmetry elements.

(a) Tetrahedral Groups: Tetrahedral carbon is fundamental to organic chemistry and many simple inorganic molecules, ions have tetrahedral symmetry. This group is denoted by T_d. A tetrahedron has four C_3 axes, three C_2 axes, six mirror planes and three S_4 improper rotational axes. It has altogether 24 symmetry operations.

(b) Octahedral Groups: Both the cube and the octahedral belong to the group labelled C. These two bodies have the same elements.

(C) Icosahedral, I_h: The pentagonal Dodecahedron and the Icosahedron are related to each other in the same way as are the Octahedron and the cube. Both have the same symmetry operations 120. The group of 120 operations is denoted by I_h which is called Icosahedral. Six C_5 axes, ten C_3 axes, 15 C_2 axes and 15 planes of symmetry. For example $B_{12}H^{2-}{}_{12}$ ion.

CONCLUSION

The subject studied here is the mathematics behind the idea of symmetry. We use the general properties of groups to aid in correctly and systematically determining the symmetry operation of any molecule. It is interesting to notice that by changing the symmetry plane of a molecule the scientists produce different drugs from the same molecules. Moreover, by studying the symmetry of different molecules one can say that whether there will be a chemical reaction between the molecule or not. Throughout this study we have realized that to study molecular symmetry the strong mathematical background is needed indeed.

REFERENCES

1. Artin, M. (2006). Algebra, New Delhi: Prentice Hall of India Original US Edition.
2. Bhagi, A, Jain, V, Raj. (2010). G, Group Theory and Symmetry in Chemistry, Meerut: Krishna Prakashan Media (P) Ltd., 3rd Edition.
3. Cotton, F. A. (1990). Chemical Applications of Group Theory, John Wiley and Sons, 3rd Edition.
4. Donalt A., John D. (2005). Physical Chemistry, Siomon Viva Books Private Ltd.
5. Gupta, B. D. (2010). Mathematical Physics¸Vikas Publishing House Pvt. Ltd. 4th Edition.
6. Jolly William L. (2000). Modern Inorganic Chemistry, New Delhi: McGrow Hill.
7. Ladd Mark (1990). Introduction to Physical Chemistry, Cambridge
8. Lesk Arthur M. (2004). Introduction to Symmetry and Group Theory for Chemists, Kluwer Academic Publishers.
9. Scholand, D. (1965). Molecular Symmetry, London: D. Van Nostrand.
10. Shriven and Atkins (2006). Inorganic Chemistry, London: Oxford University Press, International Student Edition.
11. Wikipedia (the free encyclopaedia), Molecular Symmetry.