Understanding Molecular Symmetry and Symmetry Groups

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1 Abstract:

This report delves into the concepts of molecular symmetry, symmetry elements of elements, symmetry groups, their orders and classes, and matrix representations of symmetry elements.

2 What is Molecular Symmetry?

Molecular symmetry refers to the inherent spatial arrangement and organization of atoms within a molecule, which remains unchanged under certain symmetry operations. It describes the patterns of symmetry present in a molecule due to the arrangement of its constituent atoms and the distribution of electron density.

In simpler terms, molecular symmetry deals with how the overall shape and structure of a molecule can be unchanged or transformed by various symmetry operations, such as rotation, reflection, inversion, or a combination of these operations. These symmetry operations reveal repetitive patterns or arrangements within the molecule, aiding in the understanding of its properties, behavior, and interactions with other molecules.

Understanding molecular symmetry is crucial in various fields of chemistry, including spectroscopy, crystallography, and chemical reaction mechanisms, as it provides insights into molecular properties and behavior, helping scientists predict and interpret experimental results more accurately.

3 What is Symmetry of Element?

Symmetry element is a point, line, or plane about which symmetry operation can take place. There are four types of elements of symmetry.

a) Identity (E)

Identity means basically no operation is performed. Every object possesses at least the identity element. An object having no symmetry elements other than E is called asymmetric.

b) Rotation (C_n)

Also known as radial symmetry, is represented by an axis about which it rotates in its corresponding symmetry operation. Usually, group proper rotations are denoted as C_n where the degrees of rotation that restore the object is 360°/n where n represents the number of axes.

c) Reflection plane (σ_v)

Denoted as σ, a mirror plane that includes the axis is called a vertical mirror, mirror plane and denoted as σ_v. A vertical mirror plane that bisects the angle between two C_2 axes is called "Dihedral Mirror Plane σ_d".

d) Rotational-Reflection plane (σ'_d)

Also known as improper rotation is an isometry in Euclidean space that is a combination of a rotation about an axis and a reflection in a plane perpendicular to that.

4 Symmetry elements form a group

Here we take the order of axis as 2. So, $G = (\{E, C_2, \sigma_v, \sigma'_v\}, *)$. Now we have made a multiplication table.

Table 1: Multiplication Table for a Group of 4 Elements

*	E	C_2	σ_v	σ'_v
E	E	C_2	σ_v	σ'_v
C_n	C_2	E	σ'_v	σ_v
σ_v	σ_v	σ'_v	E	C_2
σ'_v	σ'_v	σ_v	C_2	E

Now from the given table, we can say G is closed.
For all $a, b, c \in G$, $(a * b) * c = a * (b * c)$, therefore associative.
E is the identity.
For all $a \in G$, $a * a = E$, so the inverse exists.
For all $a, b \in G$, $a * b = b * a$, so commutative.
Hence G is a Commutative Group.

5 Properties of the Group Elements

We can observe the following properties of the group elements:

- $E * E = E$; $E * E * \ldots * E = E$
- $C_2 * C_2 = E$; $C_2 * C_2 * C_2 = C_2$;
  therefore $C_2 * C_2 \ldots * C_2 = \begin{cases} E & \text{when } n \text{ is even,} \\ C_2 & \text{when } n \text{ is odd} \end{cases}$
- $\sigma_v * \sigma_v = E$; $\sigma_v * \sigma_v * \sigma_v = \sigma_v$; therefore $\sigma_v * \sigma_v \ldots * \sigma_v =$
  $\begin{cases} E & \text{when } n \text{ is even,} \\ \sigma_v & \text{when } n \text{ is odd} \end{cases}$
- $\sigma'_v * \sigma'_v = E$; $\sigma'_v * \sigma'_v * \sigma'_v = \sigma'_v$; therefore $\sigma'_v * \sigma'_v \ldots * \sigma'_v =$
  $\begin{cases} E & \text{when } n \text{ is even,} \\ \sigma'_v & \text{when } n \text{ is odd} \end{cases}$

Therefore, no generator exists. Hence $G = (\{E, C_2, \sigma_v, \sigma'_v\}, *)$ is not a cyclic group.

6 Order and Class of the Group

Order
The total number of symmetry operation needed to get the original form is called order of the group.
Here order of G is 4, but order of every elements of this group is undefined.

Class
A set of element in a group that are conjugate to one another are said to form a class of a group.

7 Matrix representation of symmetry elements

$E(x, y, z) \rightarrow (x, y, z)$ To understand whether there is any rotation or asymmetry or inversion in the structure,matrix representation of symmetry elements is required.
Identity

$$E \begin{pmatrix} x \\ y \\ z \end{pmatrix} \rightarrow \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} 1 \cdot x + 0 \cdot y + 0 \cdot z \\ 0 \cdot x + 1 \cdot y + 0 \cdot z \\ 0 \cdot x + 0 \cdot y + 1 \cdot z \end{pmatrix}$$

$$E\begin{pmatrix}x\\y\\z\end{pmatrix} = \begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}\begin{pmatrix}x\\y\\z\end{pmatrix}$$

$$E = \begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}$$

Now character = sum of all principal diagonal element
If character = n for n dimension then matrix is identical.

Center of Inversion

$$i\begin{pmatrix}x\\y\\z\end{pmatrix} \rightarrow \begin{pmatrix}-x\\-y\\-z\end{pmatrix} = \begin{pmatrix}-1\cdot x+0\cdot y+0\cdot z\\0\cdot x-1\cdot y+0\cdot z\\0\cdot x+0\cdot y-1\cdot z\end{pmatrix}$$

$$i\begin{pmatrix}x\\y\\z\end{pmatrix} = \begin{pmatrix}-1&0&0\\0&-1&0\\0&0&-1\end{pmatrix}\begin{pmatrix}x\\y\\z\end{pmatrix}$$

$$i = \begin{pmatrix}-1&0&0\\0&-1&0\\0&0&-1\end{pmatrix}$$

Now character = sum of all principal diagonal element
If character = -n for n dimension then center of inversion exists.

Reflection plane

$$\sigma_{xz}\begin{pmatrix}x\\y\\z\end{pmatrix} \rightarrow \begin{pmatrix}x\\-y\\z\end{pmatrix} = \begin{pmatrix}1\cdot x+0\cdot y+0\cdot z\\0\cdot x-1\cdot y+0\cdot z\\0\cdot x+0\cdot y+1\cdot z\end{pmatrix}$$

$$\sigma_{xz}\begin{pmatrix}x\\y\\z\end{pmatrix} = \begin{pmatrix}1&0&0\\0&-1&0\\0&0&1\end{pmatrix}\begin{pmatrix}x\\y\\z\end{pmatrix}$$

$$\sigma_{xz} = \begin{pmatrix}1&0&0\\0&-1&0\\0&0&1\end{pmatrix}$$

Similarly for

$$\sigma_{xy} = \begin{pmatrix}1&0&0\\0&1&0\\0&0&-1\end{pmatrix}$$

and

$$\sigma_{yz} = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

If character = 1 $\forall$ plane then we can say it's symmetric.

Rotational-Reflexive plane

$$\sigma'_{xy} \begin{pmatrix} x \\ y \\ z \end{pmatrix} \rightarrow \begin{pmatrix} -x \\ -y \\ z \end{pmatrix} = \begin{pmatrix} -1 \cdot x + 0 \cdot y + 0 \cdot z \\ 0 \cdot x - 1 \cdot y + 0 \cdot z \\ 0 \cdot x + 0 \cdot y + 1 \cdot z \end{pmatrix}$$

$$\sigma'_{xy} \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

$$\sigma'_{xy} = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Similarly for

$$\sigma'_{yz} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

and

$$\sigma'_{xz} = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

If character = -1 $\forall$ plane then it's asymmetry.

8 conclusion

Group theory is a very fundamental thing in mathematics which are not bounded in theory but we can use it in various field to understand that subject in deeper manner.Here I am trying to understand the molecular symmetry using group theory in two dimensional space.