Groups in Molecular Symmetry

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What is Molecular Symmetry?

- ❖ It is a fundamental concept of chemistry that allows to predict or explain many of a molecule's chemical properties.
- ❖ important aspect of molecular symmetry is the concept of symmetric operation.

What is Symmetry of Element?

It's a criteria for defining a molecule is symmetry or not.

There are four types of element of symmetry. a) Identity (E).

b) Rotation (C_n) [where n denotes order of axis]

c) reflection plane (σ_v)

d) rotational-reflection plane (σ'_v)

Symmetry elements form a group

Here we take order of axis is 2. So, G= ({E, C_2 , σ_v ,σ'_v },*). Now we have made a multiplication table.

From the multiplication table we can say-

- G is closed.
- Let’s take a,b,c in G such that ∀a,b,c there exist (a*b)*c = a*(b*c). Hence associative.
- Identity exist
- For every element of the group there is an inverse.
- ∀a,b of G, a*b = b*a. Hence commutative.

Therefore G is a Commutative Group.

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

Continue...

$E*E = E$; $E*E*\ldots*E = E$

$C_2 * C_2 = E$; $C_2 * C_2 * C_2 = C_2$; therefore $C_2 * C_2 \ldots * C_2 = \begin{cases} E & \text{when n is even} \\ C_2 & \text{when n is odd} \end{cases}$

$\sigma_v * \sigma_v = E$; $\sigma_v * \sigma_v * \sigma_v = \sigma_v$;therefore $\sigma_v * \sigma_v \ldots * \sigma_v = \begin{cases} E & \text{when n is even} \\ \sigma_v & \text{when n is odd} \end{cases}$

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

Therefore no generator exists.

Hence $G= (\{E, C_2, \sigma_v, \sigma'_v\},*)$ is not a cyclic group.

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.

Class:

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

Matrix representation of symmetry elements

Identity:

E(x,y,z)⟶(x,y,z)

$$E\begin{bmatrix} X \\ Y \\ z \end{bmatrix} \longrightarrow \begin{bmatrix} X \\ Y \\ z \end{bmatrix} = \begin{pmatrix} 1.X+0.Y+0.Z \\ 0.X+1.Y+0.Z \\ 0.X+0.Y+1.Z \end{pmatrix}$$

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

Now, character = sum of principal diagonal element.

If character = n for n dimension then matrix is identical.

Continue...

Center of inversion:

$I(x,y,z) \longrightarrow (-x,-y,-z)$

$$I \begin{pmatrix} X \\ Y \\ z \end{pmatrix} \longrightarrow \begin{pmatrix} -X \\ -Y \\ -z \end{pmatrix} = \begin{pmatrix} -1.X+0.Y+0.Z \\ 0.X-1.Y+0.Z \\ 0.X+0.Y-1.Z \end{pmatrix}$$

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

Now, character = sum of principal diagonal element.

If character = -n for n dimension then center of inversion exists.

Continue...

Reflection plane:

$\sigma_{xz}(x,y,z) \longrightarrow (x,-y,z)$

$$\sigma_{xz} \begin{pmatrix} X \\ Y \\ z \end{pmatrix} \rightarrow \begin{pmatrix} X \\ -Y \\ z \end{pmatrix} = \begin{pmatrix} 1.X+0.Y+0.Z \\ 0.X-1.Y+0.Z \\ 0.X+0.Y+1.Z \end{pmatrix}$$

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

now character = sum of principal diagonal element.

If character = 1 for all plane then it's symmetry.

Continue...

Rotational-reflexive plane:

σ'_{xy} (x,y,z)⟶(-x,-y,z)

$$\sigma'_{xy} \begin{pmatrix} X \\ Y \\ z \end{pmatrix} \rightarrow \begin{pmatrix} -X \\ -Y \\ z \end{pmatrix} = \begin{pmatrix} -1.X+0.Y+0.Z \\ 0.X-1.Y+0.Z \\ 0.X+0.Y+1.Z \end{pmatrix}$$

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

now character = sum of principal diagonal element.

If character = -1 for all plane then it’s asymmetry.

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.

Thank you