Bharathidasan University
Tiruchirappalli -620 024

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Unit-I Group Theory

Dr. V. Thiagarajan
UGC-Assistant Professor
School of Chemistry

Group theory basics

Group:

A group is a set of elements along with a rule for combining them, and the elements and the rule must satisfy the following four defining properties:

(i) Closure:

The combination of any two elements from the group must result in another element that is also in the group. In other words, if **A** and **B** are elements of the group, then **A·B** (the result of combining A and B) must also be in the group.

(ii) Identity:

There must be an identity element **E** in the group such that, for any element A in the group, A· **E** = **E** ·A= A. This element does not change the other elements when combined with them.

(iii) Inverses:

For every element A in the group, there must be an inverse element $\mathbf{A}^{-1}$ such that

$A \cdot \mathbf{A}^{-1} = \mathbf{A}^{-1} \cdot A = E$, where E is the identity element.

(iv) Associativity:

The group operation must be associative, meaning that for any three elements A, B, and C, we must have $(A \cdot B) \cdot C = A \cdot (B \cdot C)$

- **Additionally:**

Commutativity:

If the group is **abelian** (commutative), then the operation must satisfy $A \cdot B = B \cdot A$.

However, if the group is **non-abelian**, the commutative law does not hold, meaning $A \cdot B \neq B \cdot A$ in general.

- **Examples:**

1. With the combining rule of **addition**, the set of **all integers** forms a **group.**

   E = 0

   A^{-1} = Negaive value of the same element

   This is an example of an **infinite group**, as there is no limit to the number of integers.

2. With the combining rule of **multiplication**, we can form a **finite group** with the set $\{i, -i, 1, -1\}$,

   where i is the imaginary unit, defined as $i^2 = -1$.

   E = 1

   The inverse of each element being its corresponding inverse under multiplication.

Non-Abelian groups: A group for which the elements do not commute is called a non-Abelian group. In such a group, the commutative law does not hold, meaning **$AB \neq BA$** in general.

Abelian groups: A group in which all the elements commute is called an Abelian group. In such a group, the commutative law holds, meaning **$AB = BA$** for all elements A and B.

Finite and infinite groups:

Groups can be either **finite** or **infinite**.

- A **finite group** has a finite number of elements.
- An **infinite group** has infinitely many elements.

The order of the symmetry group of a **nonlinear molecule** is finite. However, the order of the symmetry group of a **linear molecule** is infinite, since it includes the operation of rotation through any angle about the molecular axis.

Cyclic group: A **cyclic group** is a group in which all the elements can be generated by repeatedly applying a single operation (called a generator) to itself. In other words, the elements of a cyclic group are powers (or iterations) of a single element, typically written as $X, X^2, X^3, \ldots, X^n$

If the group is **finite**, then there exists a positive integer nn such that $X^n = E$, where E is the identity element of the group

Order of the group:

The **order** of a group refers to the number of elements in the group.

$G = \{i, -i, 1, -1\}$

Order of the group = h = 4

Group multiplication table

If there are n elements in a group G, and all of the possible n^2 products of these elements are known, then this group G is uniquely determined, and we can represent these n^2 products in a table called a **group multiplication table**.

The **group multiplication table** displays the result of multiplying any two elements of the group. Each element of the group appears both as a row and a column header, and the entries in the table show the result of the group operation (multiplication) between the corresponding row and column elements.

For example, if the elements of the group are A, B, and C, the table would show the results of multiplying A×A, A×B and A×C, and similarly for the other elements.

Symmetry Operations in Molecules:

All the symmetry operations of a molecule can be written in the form of a group multiplication table. The table represents how these symmetry operations combine with one another to form the full symmetry group of the molecule.

Rearrangement Theorem:

An important rule in group multiplication tables is called the **Rearrangement Theorem**. This theorem states that each element will appear exactly once in each row and column of the table. This reflects the property of **left** and **right inverses** in a group, ensuring that no element is repeated in any row or column. This is a key characteristic of a group, known as the **Latin square property**.

Interpretation of Group Operations:

In group theory, when the column element is A and the row element is B, the corresponding entry in the table is AB. This means that the operation of B is performed first, followed by the operation of A. The multiplication table follows the specific group operation defined for the group G.

Consider a group of order 3

G_3	E	A	B
E	E	A	B
A	A	?	?
B	B	?	?

There are two options for filling out the table AA = B or AA = E

If AA = E then the table becomes...

G_3	E	A	B
E	E	A	B
A	A	E	B
B	B	A	E

This violates the rearrangement theorem as the last two columns have elements that appear more than once.

The only solution for group G_3 is

G_3	E	A	B
E	E	A	B
A	A	B	E
B	B	E	A

Note: The group G_3 is a member of a set of groups called cyclic groups. Cyclic groups have the property of being Abelian that is all elements commute with each other.

A cyclic group is one that every element can be generated by a single element and it's powers. In this case A = A and AA = A^2 = B and AAA = A^3 =E

There are two possible groups of order 4

G_4	E	A	B	C
E	E	A	B	C
A	A	B	C	E
B	B	C	E	A
C	C	E	A	B

G_4	E	A	B	C
E	E	A	B	C
A	A	E	C	B
B	B	C	E	A
C	C	B	A	E

In the second case of G4 there is a subgroup of order 2 present.

G_2	E	A
E	E	A
A	A	E

The order of a subgroup (g) must be a divisor of the order of the main group (h), that is h/g = k, where k is an integer.