Explain: —
(a) Order of a group (b) Sub-group
(c) Similarity transformation and Conjugate
(d) Class.

Order of a group: -

The number of elements in a group is called its Order.

In a molecular point group, Order is the number of Symmetry operations possible.

In H_2O or Water molecule (C_{2v} Point group), the total number of symmetry operations are four and hence Order of this group is four.

In Ammonia molecule (NH_3) i.e C_{3v} Point group, the total number of symmetry operations are six and hence Order of the group is Six.

Or,

the total number of Symmetry operation conducted by a molecule in provided point group is called Order of a group.

Sub-group: - Smaller group that may be formed within a group are called sub-groups.

The elements of a subgroup should obey the following Conditions: —

(a) The elements of a sub group must obey all the Conditions of a group.

(b) If g represents the order of the group and s is the Order of sub group, then g/s is a natural number.

Example: -

In Case of Water molecule, C_{2v} is the point group and the followings are sub group.

(i) E

(ii) E, C_2^1

(iii) E σ_{xz}

(iv) E σ_{yz}

In ammonia molecule, C_{3v} is point group and the symmetry operations are, E, C_3^1, & C_3^2 Constitute a sub group of the Order 3.

Similarity transformation and Conjugate:-

If A and X are two elements of a group, then $X^{-1}AX$ will be equal to some elements of the group, which is B. then we have.

$$X^{-1}AX = B$$

Here element B is the similarity tranformation of A by X. the element A & B are also called as conjugate.

The properties of conjugate are:-

(i) Every element is conjugate of itself.

$$A = X^{-1}AX$$

(ii) If A is conjugate of B, then B is conjugate of A.

$$A = X^{-1}BX$$
$$B = Y^{-1}AY$$

[Where Y is the another element of the group]

(iii) If A is conjugate B and C then B & C are conjugate of each other.

Class:- A complete set of elements of a group that are conjugate to one another is called a "Class" of the group.

For NH_3 molecule of a point group C_{3v}, which goes under operations C_3^1 & C_3^2 and $\sigma_a, \sigma_b, \sigma_c$ are similar. According to similarity transformation rule,

$$\sigma_a^{-1} \cdot C_3^1 \cdot \sigma_a = \sigma_a \cdot \sigma_c = C_3^2$$

Taking $B = C_3^1$ and any operation X of the C_{3v} group, it can be seen that the similarity transformation leads, to either C_3^2 or C_3^1 and hence we say that C_3^1 & C_3^2 are similar and belongs to the same class.

Like wise σ_a, σ_b and σ_c belongs to the same class in C_{3v} point group.

Following are the classes for the point groups given:-

C_{2v}:- $E, C_2, \sigma_{xz}, \sigma_{yz}$ = 4 classes

C_{2h}:- E, C_2, σ_h, i = 4 classes

D_{3h}:- $E, C_3^1, C_3^2, C_2, C_2', C_2'', \sigma_h, S_3^1, S_3^5, \sigma_v', \sigma_v'', \sigma_v'''$

or, $E, 2C_3, 3C_2, \sigma_h, 2S_3, 3\sigma_v$ = 6 classes.

Group

A group is a Collection of elements that are interrelated according to Certain rule.

We are Concerned here with the groups formed by the Sets of Symmetry operations that may be Carried out on the molecule or Crystals.

The characteristics of a mathematical group are :-

(a) Closure
(b) Identity
(c) Inverse
(d) Association

(a) Closure :-

The product of any two elements in the group and the Square of each element must be an element in the group.

The Product of any two elements A and B Produce C. So C must be element of the group.

$$A \cdot B = C$$
$$A^2 = D$$
$$B^2 = E$$

then C, D and E must be elements of the group.

The order of Combination is Very important as AB is not necessarily equal to BA.

If $AB = BA$, the members A and B are said to 'Commute'.

and if $AB \neq BA$, the members A and B are not Commutative.

The members of the group which are Commutative from Abelian group.

(b) Identity:- One element of the group must Commute with all other elements and leave them Unchanged. This element is Called Identity and represented as E.

Identity must be present in a group

$$E \cdot A = A \cdot E = A$$
$$E \cdot B = B \cdot E = B$$

A and B are elements of the group.

(c) Inverse: -

Every member of the group must have its inverse as an member of the group.

$$A \cdot A^{-1} = A^{-1} \cdot A = E$$

(d) Association: -

Multiplication of elements of a group must be associative.

$$A (B \cdot C) = (A \cdot B) \cdot C$$

Symmetry elements of a molecule constitute a group.

Point Group: -

A Point groups is defined as a set of Symmetry operations (rotation, reflection etc.) that leave an object or molecule unchanged with all operations passing through a fixed point.

Multiplication table for C_{2v} Point group - Water (H_2O) belongs to C_{2v} Point group.