

2] Write down the conditions (Group postulates) for the symmetry elements to form a mathematical group.

A set of elements with a binary operation(*) form a group if the elements in the set obey the following rules.

Rule : 1

The product of any two elements A and B in the group combine to give the third element C, which is also an element of the group. and square of each element must be an element in the group.

$$A \times B = C$$

Rule :2

An element combines with itself to form another element of the group.

$$A \times A = E$$

Here E is the member of the same group.

Rule: 3

One element in the group must commute with all others and leave them unchanged. It is designed by E and it is usually represented as identity element.

For example,

$$AE = EA = A$$

$$BE = EB = B \quad (\text{here E is the identity element})$$

Rule : 4

Every element A of a group has an inverse A^{-1} which is also an element of the group.

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

Therefore, A^{-1} is the inverse of element A.

Similarly, A^{-1} , A and E should belong to the group G.

Rule : 5

Every element of the group obeys the associative law of combination.

$$A(BC) = (AB)C$$

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3) Define the following terms:

a) Abelian groups:

A Group is said to be abelian, if all the elements commute with each other.

Example : H_2O molecule belongs to Abelian Group.

b) Non-abelian groups:

A Group is said to be Non-abelian, if all the elements do not commute with each other.

Example : NH_3 molecule belongs to Non-abelian Group.

c) cyclic groups:

A group is said to be cyclic, if all its elements can be generated from the symmetry element. Thus A, A^2, A^3, A^n form the elements of the cyclic group.

Here $A^n = E$, the identity element.

In general, the roots of the equation $x^n - 1 = 0$ form a cyclic group.

d) Order of the group:

The total number of elements of a group is called as order of the group.

For example,

1. Water molecule C_{2v} point group.

The elements are $(E, C_2, \sigma_v', \sigma_v'')$

The order of the group is 4.

2. Ammonia molecule C_{3v} point group.

The elements are $(E, C_3, C_3^2, \sigma_v', \sigma_v'', \sigma_v''')$

The order of this group is 6.

e) sub-group:

This is a smaller group within a group. If any selection or subset of the element of a group satisfies the definition of a group, then this subset of the element is called a sub-group.

*Identity element is essentially a part of sub-group.

Example ; $\{E, C_2\}$ is a sub-group of C_{2v} point group.

4} Construct the Group Multiplication table for C_{2v} point group

A water molecule has four elements, $(E, C_2, \sigma_v', \sigma_v'')$

We can easily show that the product of any two symmetry elements is one of the four elements of the group.

Thus for instance, $C_2 \times \sigma_v' = \sigma_v''$

Proceeding this way the symmetry operations of H_2O molecule can be listed in a Group Multiplication table.

Step : 1

Water molecule has 4 symmetry elements . Hence, they are arranged in 4x4 table as follows.

	E	C_2	σ_v'	σ_v''
E				
C_2				
σ_v'				
σ_v''				

Step :2

Multiply all the symmetry elements of water molecule by E

$$E \times E = E$$

$$E \times C_2 = C_2$$

$$E \times \sigma_v' = \sigma_v'$$

$$E \times \sigma_v'' = \sigma_v''$$

Now the Group multiplication table is filled as follows

	E	C_2	σ_v'	σ_v''
E	E	C_2	σ_v'	σ_v''
C_2				
σ_v'				
σ_v''				

Step :3

Multiply all the symmetry elements of water molecule by C_2

$$C_2 \times E = C_2$$

$$C_2 \times C_2 = E$$

$$C_2 \times \sigma_v' = \sigma_v''$$

$$C_2 \times \sigma_v'' = \sigma_v'$$

Now the Group multiplication table at the end of step:3 is filled as follows

	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 ''				

Step :4

Multiply all the symmetry elements of water molecule by σ_v'

$$\sigma_v' \times E = \sigma_v'$$

$$\sigma_v' \times C_2 = \sigma_v''$$

$$\sigma_v' \times \sigma_v' = E$$

$$\sigma_v' \times \sigma_v'' = C_2$$

Now the group multiplication table at the end of step 4 is

	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 ''				

Step :5

Multiply all the symmetry elements of water molecule by σ_v''

$$\sigma_v'' \times E = \sigma_v''$$

$$\sigma_v'' \times C_2 = \sigma_v'$$

$$\sigma_v'' \times \sigma_v' = C_2$$

$$\sigma_v'' \times \sigma_v'' = E$$

Now the group multiplication table at the end of step 5 is

	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

