Solid State — Group theory

Two System are used in the notation of Molecular point group (i.e Schoenflies Symbols) and notation of Point groups for Crystal (i.e Hermann - Mauguin Symbol).

(1) Schoenflies Notions :-

It involves Molecular point groups i.e C_{nv}, C_{nh}, D_{nh}, T_d and O_h

where n is the maximum number of rotation axes.

v is the vertical mirror plane, It is stated only in the absence of horizontal mirror planes.

h is the horizontal mirror Plane

T is the tetrahedral point group

O is the Octahedral Point group

Examples:

(i) C_n denotes the presence of n-fold rotation axis in molecular point group

(ii) S_{2n} denotes the presence of only a 2n-fold rotation-reflection axis in point group.

(iii) C_{nh} denotes that both the C_n and mirror plane (or reflection plane) are perpendicular to the axis of rotation.

(iv) On the Contrary C_{nv} indicates both the C_n and mirror plane are parallel to the axis of rotation.

(2) Hermann - Mauguin Notation :-

It is used for space groups as well as Crystallographic Point gr.
It provides the maximum axis of rotation.

For example, In this notation the Number '2' is used to designate a Single 2-fold rotation axis in a point group

Note :- For example If schoenfles notation depicted as C_{2h} for a point gr. then it is represented in Hermann - Mauguin System as $2/m$ and it is read as two slash m or $2/m$

Where m denotes the mirror plane and the Slash (/) denotes that the mirror plane is perpendicular to the two-fold axis.

Lattice System	—	Point Groups		—	—	—	—
Triclinic	1	-1					
Monoclinic	2	m	$2/m$				
Tetragonal	$+4$	-4	$4/m$	422	4mm	$-42mm$	$4/mmm$
Hexagonal	6	-6	$6/m$	622	6mm	$-62mm$	$6/mmm$

In a Crystal about 230 space groups are present in 3D manner these space groups are Combination of 14 Bravias lattices and 32 Crystallographic point groups.

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Group Postulates: -

The Complete set of operations forms a mathematical group. In order that the Symmetry elements A, B, C, ... forms a mathematical group G, the following Conditions must be satisfied.

1. Two elements A and B of a group Combine to give a third element C, which is also an element of the group.

$$AB = C$$

It means that the application of B followed by A is equivalent to the application of C

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

2. An element Combines with itself to form another element of the group.

3. The group must Contain the identity element E which Commutes with all the element and leaves them unchanged.

$$EA = AE = A$$

$$EB = BE = B \quad \text{etc.}$$

4. Every element of the group obeys the associative law - of Combination

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

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

$$AA^{-1} = A^{-1}A = E$$

A Mathematical Study of Symmetry is Called Group theory.

Now we use the following methods to Simplify group representations Problem.

1. use of matrices in group representations
2. Use of Vectors in group representation
3. Use of Mathematical functions in group representations

1. Use of matrices is the most safest and accurate method to find out the each operation on the Co-ordinates.

Matrix: - A matrix is a rectangular array of numbers of Symbols Called elements that has the following general form

$$\begin{bmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{bmatrix}$$

In the above matrix the vertical sets of elements are called Columns and Horizontal is Called rows.

For example The Symbol A_{ij} means the Matrix element in the i^{th} row and in j^{th} Column.

i.e. A_{12} = Element is in 1st row and 2nd Column.

& A_{23} means the element in 2nd row and 3rd Column. etc.

When the number of row is equal to Column, then the matrix is Called Square Matrix

The element A_{ij} of a square matrix for which $i = j$ (ie A_{11}, A_{22}, A_{33}) are called the Diagonal element and except diagonal element all are Called Off diagonal.

... elements of a Square matrix equals 1 and