Reducible and Irreducible Representation

The Character of the Identity operation is the dimention of a Representation.

A representation of higher dimension which can be reduced to representation of lower dimension is known as reducible representation. And those representation which can not be further reduced to representation of lower dimension are called irreducible representation.

It is important to know the number of irreducible representation in a group. Representation of higher dimension may be reduced to matrices of smaller dimensions by a process of similarity transformation.

If A is a big matrix and it is to be reduced into B. (i.e. matrix of smaller dimension) Now we choose a Matrix X and evaluate $X^{-1}AX$ which gives us B

i.e $X^{-1}AX = B$

Where A, B and X are matrix of the same dimensions.

$$\text{If } A = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} \xrightarrow[\text{transformation } [X^{-1}AX]]{\text{Similarity}} \begin{bmatrix} b_{11} & b_{12} & 0 \\ b_{21} & b_{22} & 0 \\ 0 & 0 & b_{33} \end{bmatrix}$$

A matrix A of 3×3 dimension has been converted to two matrices one of 2×2 and the other 1×1 dimension. This similarity transformation block diagonalises the original matrix to matrices of reduced order in block form. We know transformation matrices are operators of the class to which they belong.

A matrix X does not reduce B further ($X^{-1}BX = B$), then we can say that the dimension is irreducible and its matrices can not be further reduced to lower dimension.

Irreducible representations are of prime significance in dealing with the problems associated with molecular geometry.

It is also noted that there will be as many irreducible representations for any point group as there are classes of symmetry operations for that group.

Thus, in C_{2v} point group, there are four classes and four irreducible one dimensional representations.

In C_{3v} point group, there are three classes and hence three irreducible representations.

Great Orthogonality theorem

The Orthogonality theorem is concerned with elements of matrices constituting irreducible representation of a Point group. The great orthogonality theorem in mathematical form is given below.

$$\sum_R [\Gamma_i (R)_{mn}] [\Gamma_j (R)_{m'n'}] = \frac{h}{\sqrt{l_i l_j}} \delta_{ij} \delta_{mm'} \delta_{nn'}$$

Here $\Gamma_i (R)_{mn}$ stands for the element in the mth row and nth Column of the matrix corresponding to an operation R in the ith irreducible representation.

It is necessary to take the complex conjugate (denoted by *) of one factor on the left hand side whenever imaginary or complex numbers are involved.

The complex conjugate of the element in the m'th row & n'th column of a matrix in the jth irreducible representation is denoted by $[\Gamma_j (R)_{m'n'}]^*$, l_i and l_j are the dimensions of the ith and jth irreducible representation. h is the order (total number of symmetry operations) of the point group δ_{ij}, $\delta_{mm'}$, and $\delta_{nn'}$, denote the Kronecker delta symbol.

For simplicity, we can remove the explicit designation of complex conjugate. Then the simple equation can be represented as

$$\sum_R [\Gamma_i (R)_{mn}] [\Gamma_j (R)_{mn}] = 0 \text{ if } i \neq j$$

Here, elements of corresponding matrices of different irreducible representations are orthogonal.

$$\sum_R [\Gamma_i (R)_{mn}] [\Gamma_j (R)_{m'n'}] = 0 \text{ if } m \neq m' \text{ \& } n \neq n'$$

Here, elements of different set of the matrices of the same irreducible representation are orthogonal.

$$\sum_R [\Gamma_i (R)_{mn}] [\Gamma_j (R)_{m'n'}] = \frac{h}{l_i}$$

Elements in the mth row and nth column of a matrix for operation R in the ith irreducible representation, The square of the length of any such vector equals $\frac{h}{l}$.

Consequeces of Orthogonality theorem (GOT)

Properties of irreducible representation: The properties of irreducible representation are essential to construct the character table of point group.

The following five properties are for the irreducible representation.

(i) The number of irreducible representation of a group is equal to the number of classes in the group.

(ii) The sum of the squares of the dimension of the irreducible representation of a group is equal, to the order of the group.

$$\sum l_i^2 = l_1^2 + l_2^2 + l_3^2 + \cdots = h$$

Since $\chi_i(E)$, the character of the representation of identity operation (E) in the i^{th} irreducible representation is equal to the order of representation.

We can also write as:

$$\sum_i [\chi_i(E)]^2 = h$$

(iii) The sum of the square of the character of any irreducible representation is equal to h.

$$\sum_R [\chi_i(R)]^2 = h$$

(iv) The character of two different irreducible representations of the same group are orthogonal to each other.

$$\sum_R [\chi_i(R)\,\chi_j(R)] = 0 \quad \text{when } i \neq j$$

(v) The character of all matrices belonging to operations in the same class are identical.

So by using these rules we can construct character table of various point groups.