4.10 Reducible and Irreducible Representation

The character of the identity operation is the dimension of a representation. Above representation is a three dimensional representation.

A representation of higher dimension which can be reduced tp representation of lower dimension is called reducible representation. Those representation which cannot be further reduced to representation of lower dimension are called irreducible representation. In group theory, one is interested in knowing the number of irreducible representation in a group.

Representation of higher dimension may be reduced to matrices of smaller dimension by a process of similarity transformation. If A is a big matrix and is to be reduced to B, a matrix of smaller dimension. We choose a matrix X and evaluate $X^{-1}AX$ which gives us B.

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

A, B and X matrices are 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 say that the dimension is irreducible and its matrices can not be further reduced to lower dimension.

Irreducible representations which 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}, there are four classes and four irreducible one dimensional representation and in C_{3v}, three classes and hence three irreducible representation.

4.11 The Great Orthogonality Theorem and its Consequences

The orthogonality theorem is concerned with elements of matrices constituting irreducible representation of a point group. The great orthogonality theorem in mathematical form is as follows :

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

$\Gamma_i(R)_{mn}$ is denoted for the element in the *m*th row and the *n*th column of the matrix corresponding to an operation *R* in the *i*th 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 and *n'*th column of a matrix in the *j*th irreducible representation is denoted by $[\Gamma_j(R)_{m'n'}]^*$ l_i and l_j are the dimension of the *i*th and *j*th irreducible representation. *h* is the order (total number of symmetry operations) of the point group δ_{ij}, $\delta_{mm'}$, $\delta_{nn'}$ denote the kronecker delta symbol.

For simplicity we can omit the explict designation of complex conjugate. Then simple equations can be represented as :

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

Elements of corresponding matrices of different irreducible representation are orthogonal.

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

Elements of different set of the matrices of the same irreducible representation are orthogonal

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

Elements in the *m*th ros and *n*th column of a matrix for operation *R* in the *i*th irreducible representation. The square of the length of any such vector equals $\frac{h}{l}$.

Consequences of orthogonality theorem (Properties of irreducible representation) :

The properties of irreducible representation is essential to construct the character talls of a point group. The following fine rules are given below about 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 square of the dimension of the irreducible representation of a group is equal to the order of the group.

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

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 :

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

(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 characters of two different irreducible representations of the same group are orthogonal to each other.

$$\sum_R \chi_i(R)\cdot\chi_j(R) = 0 \qquad \text{when } i \neq j$$

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

By using these rules we can construct character table of different point group.