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M.Sc. II SEM

SYMMETRY AND GROUP THEORY

- Brief and Intensive Notes
- Multiple Choice Questions

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CHEMISTRY

Symmetry and Group Theory

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SYLLABUS

Symmetry elements and symmetry operation, definitions of group, subgroup, relation between orders of a finite group and its subgroup.

Conjugacy relation and classes. Point symmetry group. Schonflies symbols, representations of groups of matrices (representation for the Cn, Cnv, Cnh, Dnh etc. groups to be worked explicitly).

Character of a representation. The great orthogonality theorem (without proof) and its importance.

Character tables and their use; spectroscopy.

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Brief Notes

Groups & Subgroups

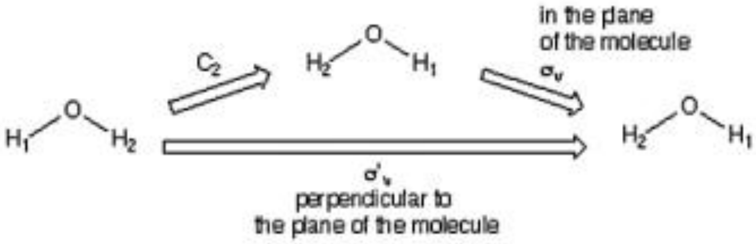
Each molecule has a set of symmetry operations that describes the molecule's overall symmetry. This set of operations define the group of the molecule.A group $G$is a finite or infinite set of elements together with a binary operation (called the group operation) that together satisfy the four fundamental properties of closure, associativity, the identity property, and the inverse property. The operation with respect to which a group is defined is often called the "group operation," and a set is said to be a group "under" this operation.

The study of groups is known as group theory.

A group is a set of operations which satisfies the following requirements-

1. Any result of two or more operations must produce the same result as application of one operation within the group.i.e., the group multiplication table must be closed

Consider H_2O which has E, C_2 and 2 σ_v's.



i.e., $\hat{C}_2\hat{\sigma}_v \equiv \hat{\sigma}'_v$ **of course** $\hat{C}_2\hat{C}_2 \equiv \hat{E}$ **etc…**
The table is closed, i.e., the results of two operations is an operation in the group i;e the elements are commutable.

2. Must have an identity ($\hat{E}$) such that AE = EA = A for any operation A in the group.

3. All elements must have an inverse i.e., for a given operation ($\hat{A}$) there must exist an operation ($\hat{B}$) such that $\hat{A}\hat{B}=\hat{E}$ or $AA^{-1} = A^{-1}A = E$
4. Each element has follows associative law

P(QR) = (PQ)R

example, the point group for the water molecule is C_{2v}, with symmetry operations E, C_2, σ_v and σ_v'. Its order is thus 4. Each operation is its own inverse. As an example of closure, a C_2 rotation followed by a σ_v reflection is seen to be a σ_v' symmetry operation: $\sigma_v * C_2 = \sigma_v'$.

The group multiplication table obtained is therefore for water molecule:

	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

$\sigma_v . \sigma_v = E$

$C_2 . \sigma_v = \sigma'_v$

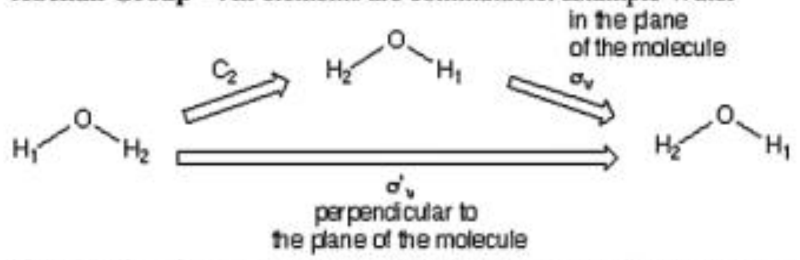
$C_2 . E = E\, C_2 = C_2$

$C_2 (\sigma_v . \sigma'_v) = (C_2 . \sigma_v) \sigma'_v$

Another example is the ammonia molecule, which is pyramidal and contains a three-fold rotation axis as well as three mirror planes at an angle of 120° to each other. Each mirror plane contains an N-H bond and bisects the H-N-H bond angle opposite to that bond. Thus ammonia molecule belongs to the C_{3v} point group which has order 6: an identity element E, two rotation operations C_3 and C_3^2, and three mirror reflections σ_v, σ_v' and σ_v''.

Classification Of Group

1. **Abelian Group –** All elements are commutable. Example Water



2. **Non Abelian Group**- All elements do not commute with one another.

Example - Phosphine symmetry operations are $E, C_1^3, C_3^4, \sigma_v^1, \sigma_v^2$

$C_3 . \sigma_v \neq \sigma_v . C_3$

3.**Cyclic group**- In cyclic group all the elements of a group can be generated from one element .It is denoted by A^n. A represents identity element & n represents total no of elements & is called as order of group. Each cyclic group is abelian but each abelian group is not cyclic.
Example Trans 1,2 dichlorocyclopropane.

Classification of group on the basis of element-

1.Monoid - A group is a monoid each of whose elements is invertible.
2. Trivial Group- A group must contain at least one element, with the unique (up to isomorphism) single-element group known as the trivial group.
3. Finite group - If there are a finite number of elements, the group is called a finite group

Subgroups

Any subset of element which form a group is called as subgroup.

A subgroup is a subset H of group elements of a group G that satisfies the four group requirements. It must therefore contain the identity element. "H is a subgroup of G" is written $H \subseteq G$, or sometimes $H \leq G$. A subset of a group that is closed under the group operation and the inverse operation is called a subgroup.

The elements of a subgroup should obey the following conditions-If g is the order of the group & s is the order of the subgroup ,then g/s is a natural number. Example- water molecule has symmetry elements- $E, C_2, \sigma_v, \sigma_v^1$

GROUP - $E, C_2, \sigma_v, \sigma_v^1$

SUBGROUPS - E

E, C_2

E, σ_v

E, σ_v^1

CLASSES – This is the subdivision of a group.

Two elements A & B in a group form a class if they are conjugate to each other. Conjugate elements are related by the equation

$$X\text{-}1AX = B$$

Where X is similarity transformation element .It is used to find whether a set of elements form a class.

Example- water molecule has symmetry elements- $E, C_2, \sigma_v, \sigma_v^1$

GROUP - $E, C_2, \sigma_v, \sigma_v^1$

CLASSES - $E^{-1} C_2 E = C_2$

$\sigma_v^{-1} C_2 \sigma_v = C_2$

$\sigma_v^{-1} C_2 \sigma_v^1 = C_2$

$C_2^{-1} C_2 C_2 = C_2$

ORDER- The order of a class of a group must be an integral factor of the order of a group and the number of elements is called the group order of the group.

Method to find the class –

1.Symmetry operations which commutes with all symmetry operations forms a class.

E, σ_h, I belongs to separate class

2.Rotation operation & its inverse forms a class like C_2^{-1} & C_2

3. Improper axis & inverse forms a class $S_1 S_1^{-1.}$

4. Two rotation about different axis forms a class if there is a third operation which interchange the points of the axis.

5. Two reflection about different planes belongs to the same class if there is a third operation which interchange points on the two plane.

Example- Square Planar AB_4 molecule has

Symmetry operations- 16- $E, i, \sigma_h, C_2^1\ C_4^1\ C_4^3\ S_4^1\ S_4^3\ 4C_2^1 4\ \sigma_v$

No Of Elements - 13

Classes- (i) E, i, σ_h, C_2 (iv) $2\ C_2^1$ operations about C_2 axis (reflection)

(ii) $C_4^1\ C_4^3$ (v) $2\ C_2^1$ operations about C_2' axis (reflection)

(iii) $S_4^1\ S_4^3$ (vi) 2 reflection operations in two σ_v planes

(vii) 2 reflection operations in two σ'_v planes

- Relation between orders of a finite group & its subgroup –

If there are a finite number of elements, the group is called a finite group and the number of elements is called the group order of the group.

- A subset of a group that is closed under the group operation and the inverse operation is called a subgroup. Subgroups are also groups, and many commonly encountered groups are in fact special subgroups of some more general larger group.
- A finite group is a group having finite group order. Examples of finite groups are the modulo multiplication groups, point groups, cyclic groups, dihedral groups, symmetric groups, alternating groups, and so on.
- The finite (cyclic) group C_2 forms the "Finite Simple Group of Order 2"
- A basic example of a finite group is the symmetric group S_n, which is the group of permutations (or "under permutation") of n objects.

Symmetry Elements & symmetry operation -

The term symmetry implies a structure in which the parts are in harmony with each other, as well as to the whole structure i;e the structure is proportional as well as balanced.

Clearly, the symmetry of the linear molecule A-B-A is different from A-A-B. In A-B-A the A-B bonds are equivalent, but in A-A-B they are not. However, important aspects of the symmetry of H_2O and CF_2Cl_2 are the same. This is not obvious without Group theory.

Symmetry Elements - These are the geometrical elements like line, plane with respect to which one or more symmetric operations are carried out.

- The symmetry of a molecule can be described by 5 types of symmetry elements. **Symmetry axis**: an axis around which a rotation by $\frac{360°}{n}$ results in a molecule indistinguishable from the original. This is also called an *n*-fold **rotational axis** and abbreviated C_n. Examples are the C_2 in water and the C_3 in ammonia. A molecule can have more than one symmetry axis; the one with the highest *n* is called the **principal axis**, and by convention is assigned the z-axis in a Cartesian coordinate system.
- **Plane of symmetry**: a plane of reflection through which an identical copy of the original molecule is given. This is also called a mirror plane and abbreviated σ. Water has two of them: one in the plane of the molecule itself and one perpendicular to it. A symmetry plane parallel with the principal axis is dubbed *vertical* (σ_v) and one perpendicular to it *horizontal* (σ_h). A third type of symmetry plane exists: if a vertical symmetry plane additionally bisects the angle between two 2-fold rotation axes perpendicular to the principal axis, the plane is dubbed dihedral (σ_d). A symmetry plane can also be identified by its Cartesian orientation, *e.g.*, (xz) or (yz).
- **Centre of symmetry** or **inversion center**, *i*. A molecule has a center of symmetry when, for any atom in the molecule, an identical atom exists diametrically opposite this center an equal distance from it. There may or may not be an atom at the center. Examples are xenon tetrafluoride (XeF_4) where the inversion cente is at the Xe atom, and benzene (C_6H_6) where the inversion center is at the center of the ring.
- **Rotation-reflection axis**: an axis around which a rotation by $\frac{360°}{n}$, followed by a reflection in a plane perpendicular to it, leaves the molecule unchanged. Also called an *n*-fold **improper rotation axis**, it is abbreviated S_n, with *n* necessarily even. Examples are present in tetrahedral silicon tetrafluoride, with three S_4 axes, and the staggered conformation of ethane with one S_6 axis.
- **Identity**, abbreviated to E, from the German 'Einheit' meaning Unity. This symmetry element simply consists of no change: every molecule has this element. It is analogous to multiplying by one (unity).

Symmetry Operations/Elements

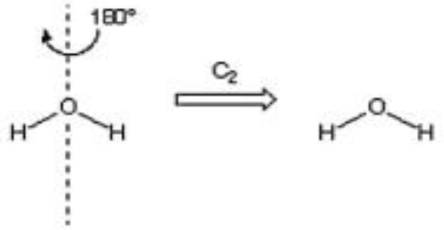
A molecule or object is said to possess a particular operation if that operation when applied leaves the molecule unchanged. Each operation is performed relative to a point, line, or plane - called a symmetry element. There are 5 kinds of operations -

1. Identity
2. n-Fold Rotations
3. Reflection
4. Inversion
5. Improper n-Fold Rotation

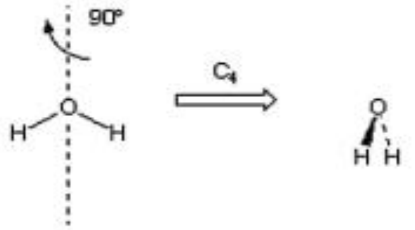
1. Identity is indicated as E

- does nothing, has no effect i;e this operation brings back the molecule to the original orientation
- all molecules/objects possess the identity operation, i.e., posses E.
- E has the same importance as the number 1 does in multiplication (E is needed in order to define inverses).

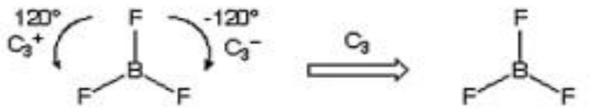
2. **n-Fold Rotations**: C_n, where n is an integer, rotation by 360°/n about a particular axis defined as the n-fold rotation axis.
C_2 = 180° rotation, C_3 = 120° rotation, C_4 = 90° rotation, C_5 = 72° rotation, C_6 = 60° rotation, etc.
Rotation of H_2O about the axis shown by 180° (C_2) gives the same molecule back.
Therefore H_2O possess the C_2 symmetry element.

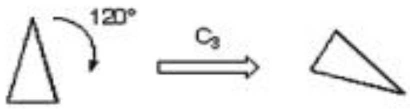


However, rotation by 90° about the same axis does not give back the identical molecule
Therefore H_2O does not possess a C_4 symmetry axis.

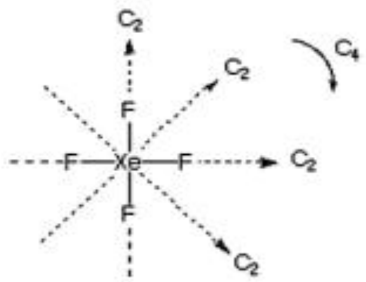


BF_3 posses a C_3 rotation axis of symmetry.



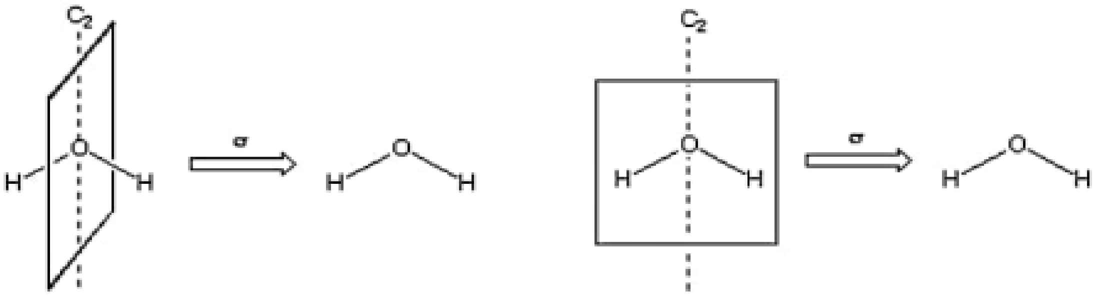


This triangle does not posses a C_3 rotation axis of symmetry.

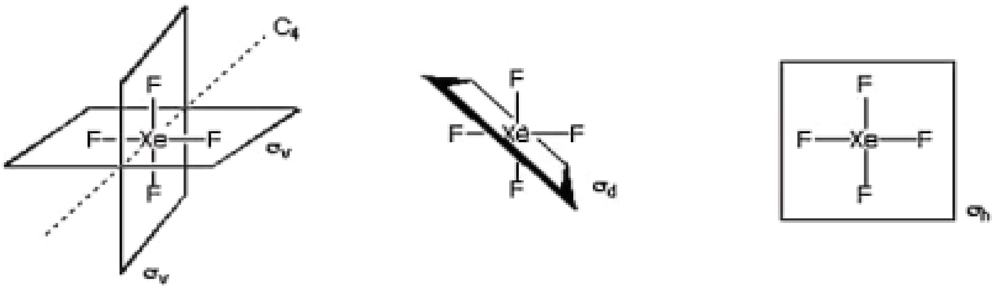


XeF_4 is square planar. It has four DIFFERENT C_2 axes . It also has a C_4 axis coming out of the page called the principle axis because it has the largest n. By convention, the principle axis is in the z-direction

3. Reflection: σ (the symmetry element is called a mirror plane or plane of symmetry)
If reflection about a mirror plane gives the same molecule/object back than there is a plane of symmetry (σ).
If plane contains the principle rotation axis (i.e., parallel), it is a vertical plane (σ_v)
If plane is perpendicular to the principle rotation axis, it is a horizontal plane (σ_h)
If plane is parallel to the principle rotation axis, but bisects angle between 2 C_2 axes, it is a diagonal plane (σ_d)
H_2O posses 2 σ_v mirror planes of symmetry because they are both parallel to the principle rotation axis (C_2)

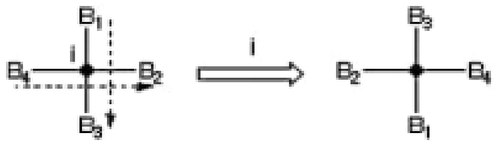


XeF$_4$ has two planes of symmetry parallel to the principle rotation axis: σ_v
XeF$_4$ has two planes of symmetry parallel to the principle rotation axis and bisecting the angle between 2 C_2 axes : σ_d
XeF$_4$ has one plane of symmetry perpendicular to the principle rotation axis: σ_h



4. Inversion: i (the element that corresponds to this operation is a center of symmetry or inversion center) .

The operation is to move every atom in the molecule in a straight line through the inversion center to the opposite side of the molecule.

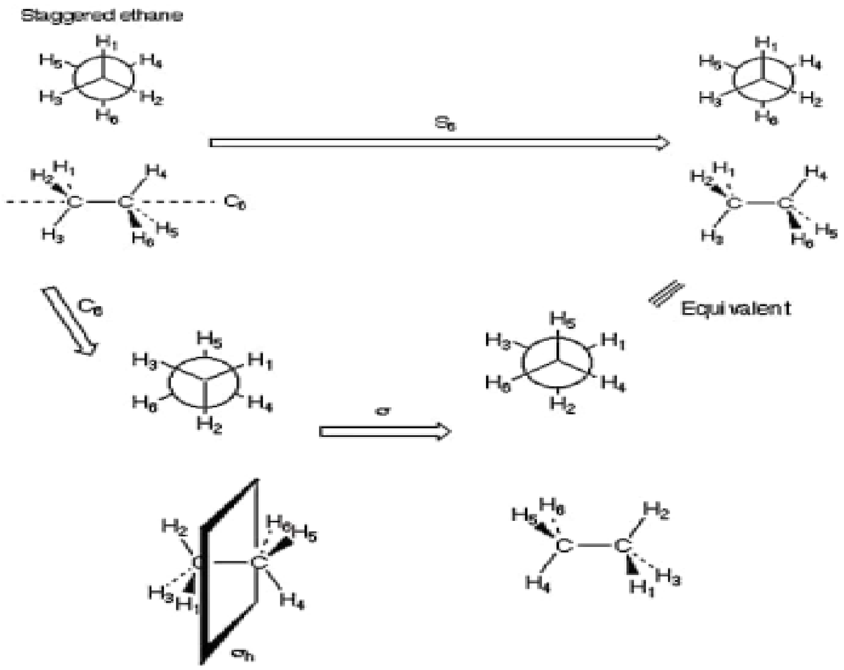


Therefore XeF$_4$ posses an inversion center at the Xe atom.

5. Improper Rotations: S_n

n-fold rotation followed by reflection through mirror plane perpendicular to rotation axis also known as Rotation Reflection axis. It is an imaginary axis passing through the molecule, on which when the molecule is rotated by $2\pi/n$ angle & then reflected on a plane perpendicular to the rotation axis then an equivalent orientation is observed.

Note: n is always 3 or larger because $S_1 = \sigma$ and $S_2 = i$.



These are different, therefore this molecule does not posses a C_3 symmetry axis.
This molecule posses the following symmetry elements: C_3, 3 σ_d, i, 3 $\perp C_2$, S_6. There is no C_3 or σ_h.
Eclipsed ethane posses the following symmetry elements: C_3, $3\sigma_v$, 3 $\perp C_2$, S_3, σ_h. There is no S_6 or i.

Compiling all the symmetry elements for staggered ethane yields a Symmetry Group called D_{3d}.

Compiling all the symmetry elements for eclipsed ethane yields a Symmetry Group called D_{3h}.

Importance of symmetry-

- It is an important concept in crystal morphology,crystal structure analysis.
- It helps in the classification of electronic states in a molecule.
- It is also useful in determining which atomic orbitals can combine to form molecules.
- It can be used in predicting the no of d-d absorption bands that are observed in coordination compounds.
- Ligand theory also depends on concept of symmetry.
- IR & Raman Spectroscopy used for structure illucidation also depends on symmetry.

Conjugacy Relation & Class

A complete set of mutually conjugate group elements. Each element in a group belongs to exactly one class, and the identity element ($I = 1$) is always in its own class. The conjugacy class orders of all classes must be integral factors of the group order of the group.

- A group of prime order has one class for each element.
- In an Abelian group, each element is in a conjugacy class by itself.
- Two operations belong to the same class when one may be replaced by the other in a new coordinate system which is accessible by a symmetry operation . These sets correspond directly to the sets of equivalent operations.
- Two elements A & B in a group form a class if they are conjugate to each other.Conjugate elements are related by the equation

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

  Where X is similarity transformation element .It is used to find whether a set of elements form a class.
- conjugacy is an equivalence relation. Also note that conjugate elements have the same order. The set of all elements conjugate to a is called the class of a.
- To find conjugacy class similarity transformations $X^{-1}\,A\,X = X^{-1}\,(A\,X)$on A. Applying a similarity transformation gives

$$A^{-1}\,D\,A = E \quad (6)$$

$$B^{-1}\,D\,B = E \quad (7)$$

$$C^{-1}\,D\,C = E \quad (8)$$

$$D^{-1}\,D\,D = D \quad (9)$$

$$E^{-1}\,D\,E = D. \quad (10)$$

10

so $\{D, E\}$form a conjugacy class.

Point Symmetry Groups - Each molecule has a set of symmetry operations that describes the molecule's overall symmetry. This set of operations define the **point group** of the molecule. Since all the elements of symmetry present in the molecule intersect at a common point & this point remains fixed under all symmetry operations of the molecule and is known as point symmetry groups.

Schonflies notation

The point groups are denoted by their component symmetries. There are a few standard notations used by crystallographers. The **Schoenflies notation** or **Schonflies notation**, named after the German mathematician Arthur Moritz Schoenflies, is one of two conventions commonly used to describe crystallographic point groups. This notation is used in spectroscopy. The other convention is the Hermann-Mauguin notation, also known as the International notation. A point group in the Schoenflies convention is completely adequate to describe the symmetry of a molecule; this is sufficient for spectroscopy. The Hermann-Maunguin notation is able to describe the space group of a crystal lattice, while the Schoenflies notation isn't. Thus the Hermann-Mauguin notation is used in crystallography.

Schönflies notation

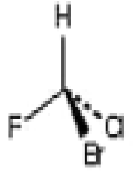
In Schönflies notation, point groups are denoted by a letter symbol with a subscript. The symbols used in crystallography mean the following:

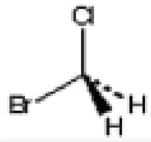
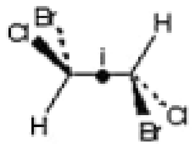
- The letter *O* (for octahedron) indicates that the group has the symmetry of an octahedron (or cube), with (O_h) or without (*O*) improper operations .
- The letter *T* (for tetrahedron) indicates that the group has the symmetry of a tetrahedron. T_d includes improper operations, *T* excludes improper operations, and T_h is *T* with the addition of an inversion.
- The letter *I* (for icosahedron) indicates that the group has the symmetry of an icosahedron (or dodecahedron), either with (I_h) or without (*I*) improper operations.
- C_n (for cyclic) indicates that the group has an *n*-fold rotation axis. C_{nh} is C_n with the addition of a mirror (reflection) plane perpendicular to the axis of rotation. C_{nv} is C_n with the addition of a mirror plane parallel to the axis of rotation.
- S_n (for *Spiegel*, German for mirror) denotes a group that contains only an *n*-fold rotation-reflection axis.
- D_n (for dihedral, or two-sided) indicates that the group has an *n*-fold rotation axis plus a twofold axis perpendicular to that axis. D_{nh} has, in addition, a mirror plane perpendicular to the *n*-fold axis. D_{nv} has, in addition to the elements of D_n, mirror planes parallel to the *n*-fold axis.

Point Groups

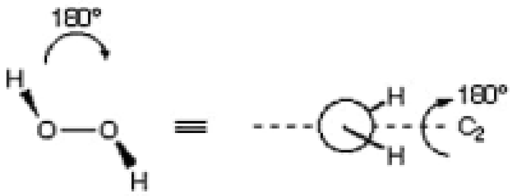
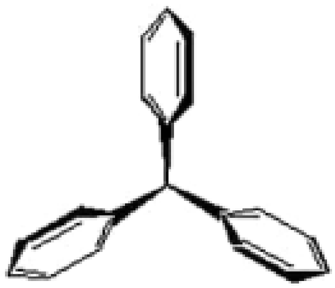
Low Symmetry Groups

C_1: only E

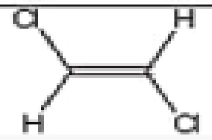


C_s: E and σ only

C_i: E and i only


C_n, C_{nv}, C_{nh} Groups

C_n: E and C_n only
C_2:

C_3:


C_{nv}: E and C_n and n σ_v's
C_{2v}: E, C_2, 2 σ_v H_2O **C_{3v}**: E, C_3, 3 σ_v NH_3 **$C\sigma_v$**: E, C , σ_v HF, HCN
C_{nh}: E and C_n and σ_h (and others as well)
C_{2h}: E, C_2, σ_h, I

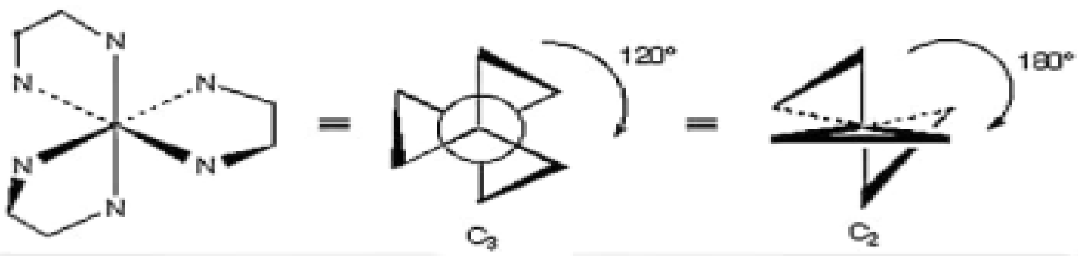


D_n, D_{nv}, D_{nh} Groups

D_n: E, C_n, n C_2 axes to C_n

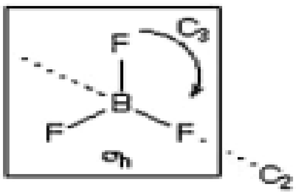
D_3: E, C_3, 3 C_2

$[Co(en)_3]^{3+}$



D_{nh}: E, C_n, n C_2 axes , σ_h

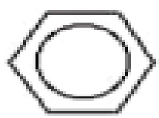
D_{3h}: E, C_3, 3 C_2, σ_h



D_{3h}: E, C_3, 3 C_2, σ_h

eclipsed ethane

D_{6h}: E, C_6, 6 C_2, σ_h



D h: E, C , C_2, σ_h

O=C=O

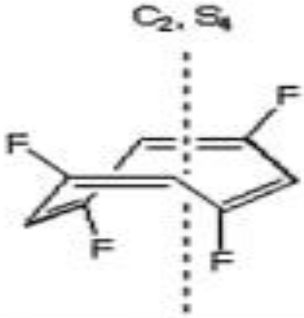
H_2

D_{nd}: E, C_n, n C_2 axes ⊥ to C_n,

D_{3d}: E, C_3, 3 C_2, 3 σ_d

staggered ethane

S_n Group

S_{2n}: E, C_n, S_{2n} (no mirror planes) S_4, S_6, S_8, etc. (Note: never S_3, S_5, etc.)
S_4: E, C_2, S_4 

High Symmetry Cubic Groups, T_d, O_h, I_h

T_d: E, 8 C_3, 3 C_2, 6 S_4, 6 σ_d Tetrahedral structures No need to identify all the symmetry elements - simply recognize T_d shape. methane, CH_4
O_h: E, 8 C_3, 6 C_2, 6 C_4, i, 6 S_4, 8 S_6, 3 σ_h, 6 σ_d Octahedral structures No need to identify all the symmetry elements - simply recognize O_h shape. 
I_h: E, 12 C_5, 20 C_3, 15 C_2, i, 12 S_{10}, 20 S_6, 15 σ Icosahedron
Other rare high symmetry groups are **T**, **T_h**, **O**, and **I**

Common point groups

Point group	Symmetry elements	**Simple description**, chiral if applicable	**Illustrative species**
C_1	E	no symmetry, chiral	CFClBrH, lysergic acid
C_s	E σ_h	planar, no other symmetry	thionyl chloride, hypochlorous acid
C_i	E *i*	Inversion center	*anti*-1,2-dichloro-1,2-dibromoethane
$C_{\infty v}$	E $2C_\infty$ σ_v	Linear	hydrogen chloride, dicarbon monoxide
$D_{\infty h}$	E $2C_\infty$ $\infty\sigma_i$ *i* $2S_\infty$ ∞C_2	linear with inversion center	dihydrogen, azide anion, carbon dioxide
C_2	E C_2	"open book geometry," chiral	hydrogen peroxide
C_3	E C_3	propeller, chiral	triphenylphosphine
C_{2h}	E C_2 *i* σ_h	planar with inversion center	trans-1,2-dichloroethylene
C_{3h}	E C_3 C_3^2 σ_h S_3 S_3^5	Propeller	Boric acid
C_{2v}	E C_2 $\sigma_v(xz)$ $\sigma_v'(yz)$	angular (H_2O) or see-saw (SF_4)	water, sulfur tetrafluoride, sulfuryl fluoride
C_{3v}	E $2C_3$ $3\sigma_v$	trigonal pyramidal	ammonia, phosphorus oxychloride
C_{4v}	E $2C_4$ C_2 $2\sigma_v$ $2\sigma_d$	square pyramidal	xenon oxytetrafluoride
T_d	E $8C_3$ $3C_2$ $6S_4$ $6\sigma_d$	tetrahedral	methane, phosphorus pentoxide, adamantane
O_h	E $8C_3$ $6C_2$ $6C_4$ $3C_2$ *i* $6S_4$ $8S_6$ $3\sigma_h$ $6\sigma_d$	octahedral or cubic	cubane, sulfur hexafluoride
I_h	E $12C_5$ $12C_5^2$ $20C_3$ $15C_2$ *i* $12S_{10}$ $12S_{10}^3$ $20S_6$ 15σ	icosahedral	C_{60}, $B_{12}H_{12}^{2-}$

Method of determination of point group of molecules- The process used to assign a molecule to a point group is straightforward with a few exceptions. It is a procedure. Here are set of steps to quickly guide you.

1. Look at the molecule and see if it seems to be very symmetric or very unsymmetric. If so, it probably belongs to one of the special groups (**low symmetry:** C_1, C_s, C_i or linear $C_{\infty v}$, $D_{\infty h}$) or high symmetry (T_d, O_h, I_h..).
2. For all other molecules find the rotation axis with the highest n, the highest order **Cn** axis of the molecule.
3. Does the molecule have any $\mathbf{C_2}$ axes **perpendicular to** the $\mathbf{C_n}$ axis? If it does, there will be n of such C_2 axes, and the molecule is in one of **D** point groups. If not, it will be in one of **C** or **S** point groups.

Does it have any mirror plane (σ_h) perpendicular to the C_n axis? If so, it is $\mathbf{C_{nh}}$ or D_{nh}.

Does it have any mirror plane (σ_d,σ_v)? If so, it is C_{nv} or D_{nd}

Representation of groups by matrices-

Group actions, and in particular representations, are very important in group theory, & Also to physics and chemistry. Since a group can be thought of as an abstract mathematical object, the same group may arise in different contexts. It is therefore useful to think of a representation of the group as one particular incarnation of the group, which may also have other representations. Any symmetry operation about a symmetry element in a molecule involves the transformation of a set of coordinates x,y,z of an atom into a set of new coordinates x',y',z'.

$$\begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

The two sets of coordinates can be related by a set of equation which is formulated in matrix notation. Thus each symmetry operation can be represented by special matrix which helps to solve structural problems in chemistry.

Matrix representation of symmetry operations- The matrices for the different symmetry operations can be obtained by considering the effect of these operations on the components of a two dimensional vector. The results can be extended to3 dimensions.

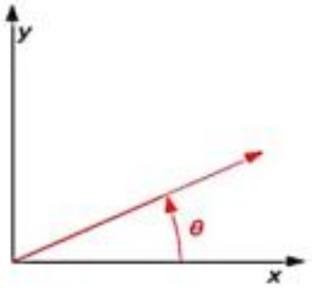
Rotations in two dimensions

Matrix representation for the Rotation operation – For 2D coordinate system X & Y , there is a vector r which can be represented by column matrix.

The symmetry operations can be **represented in many ways**. A convenient representation is by **matrices**. For any vector representing a point in Cartesian coordinates, left-multiplying it gives the new location of the point transformed by the symmetry operation. Composition of operations corresponds to matrix multiplication. In the C_{2v} example this is:

$$\underbrace{\begin{bmatrix}-1 & 0 & 0\\ 0 & -1 & 0\\ 0 & 0 & 1\end{bmatrix}}_{C_2} \times \underbrace{\begin{bmatrix}1 & 0 & 0\\ 0 & -1 & 0\\ 0 & 0 & 1\end{bmatrix}}_{\sigma_v} = \underbrace{\begin{bmatrix}-1 & 0 & 0\\ 0 & 1 & 0\\ 0 & 0 & 1\end{bmatrix}}_{\sigma_v'}$$

Although an infinite number of such representations exist, the irreducible representations (or "irreps") of the group are commonly used, as all other representations of the group can be described as a linear combination of the irreducible representations.



A counterclockwise rotation of a vector through angle θ. The vector is initially aligned with the x-axis.In two dimensions every rotation matrix has the following form:

$$R(\theta) = \begin{bmatrix}\cos\theta & -\sin\theta\\ \sin\theta & \cos\theta\end{bmatrix}$$

This rotates column vectors by means of the following matrix multiplication:

$$\begin{bmatrix}x'\\ y'\end{bmatrix} = \begin{bmatrix}\cos\theta & -\sin\theta\\ \sin\theta & \cos\theta\end{bmatrix}\begin{bmatrix}x\\ y\end{bmatrix}$$

So the coordinates (x',y') of the point (x,y) after rotation are:

$$x' = x\cos\theta - y\sin\theta,$$
$$y' = x\sin\theta + y\cos\theta.$$

The direction of vector rotation is counterclockwise if θ is positive (e.g. 90°), and clockwise if θ is negative (e.g. -90°).

$$R(-\theta) = \begin{bmatrix}\cos\theta & \sin\theta\\ -\sin\theta & \cos\theta\end{bmatrix}$$

Common rotations

If C_n represents rotation about the axis by angle θ

r = C_n X r where C_n = R (-θ)

Particularly useful are the matrices for 90° and 180° rotations:

$$R(90°) = \begin{bmatrix}0 & -1\\ 1 & 0\end{bmatrix}$$ (90° counterclockwise rotation)

For C_2, θ= 180^0

$$R(180°) = \begin{bmatrix}-1 & 0\\ 0 & -1\end{bmatrix}$$ (180° rotation in either direction – a half-turn)

$$R(270^\circ) = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}$$ (270° counterclockwise rotation, the same as a 90° clockwise rotation)

Rotations in three dimensions

$$R_x(\theta) = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos\theta & -\sin\theta \\ 0 & \sin\theta & \cos\theta \end{bmatrix}$$

$$R_y(\theta) = \begin{bmatrix} \cos\theta & 0 & \sin\theta \\ 0 & 1 & 0 \\ -\sin\theta & 0 & \cos\theta \end{bmatrix}$$

$$R_z(\theta) = \begin{bmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{bmatrix}.$$

Each of these basic vector rotations typically appears counter-clockwise when the axis about which they occur points toward the observer, and the coordinate system is right-handed. R_z, for instance, would rotate toward the y-axis a vector aligned with the x-axis. This is similar to the rotation produced by the above mentioned 2-D rotation matrix.

2.Matrix for Reflection operation- Reflection on the xy-plane (analogous to a horizontal plane σ_h), coordinate z changes the sign.

$$\sigma_z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

$$\begin{pmatrix} x \\ y \\ -z \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

The matrices which are applied for performing a reflection on the yz-plane and xz-plane are the matrices σ_x and σ_y respectively.

$$\sigma_x = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} \qquad \sigma_y = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

3.Matrix for the inversion *i* operation- It relates the coordinates (x,y,z) with (-x,-y,-z) and is connected with the following matrix:

$$i = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

a two fold application of the inversion matrix yields the coordinates of the initial point (x,y,z) which is reflected by ***E = i*i***.

$$i \cdot i = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}\begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} = E$$

4.Matrix for rotatory reflection $S_n(z)$ multiply the matrices for the fundamental operations σ_z and C_n.

$$S_n(z) = \sigma_z C_n = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}\begin{pmatrix} \cos 2\pi/n & \sin 2\pi/n & 0 \\ -\sin 2\pi/n & \cos 2\pi/n & 0 \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} \cos 2\pi/n & \sin 2\pi/n & 0 \\ -\sin 2\pi/n & \cos 2\pi/n & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

5. Identity matrices- The most primitive symmetry operation is the identity and yields a final vector identical to the initial vector. It is the **unity matrix** or **identity matrix** which leaves all coordiates unaffected.

$$E = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Character of a Representation

The set of matrices for the various symmetry operations of a point group forms a representation. The set of vectors of the coordinate system,with respect to which the matrices are defined is called the basis of the representation

Example - C_{2h} point group

Four symmetry operation - E, $\mathbf{C_2}$, $\boldsymbol{\sigma_{xy}}$,**i**

Matrix representation -

$$\underbrace{\begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix}}_{C_2} \times \underbrace{\begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix}}_{\sigma_v} = \underbrace{\begin{bmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}}_{\sigma_v'}$$

Reducible & Non reducible representation –

Reducible representation – A representation of higher dimension which can be reduced to representation of lower dimension is called reducible representation.

A reduclble representation & its reduction can be understood by carrying out a similarity transformation .Suppose A,B,C, D is a representation of a group in which [B] [C] = [D].If only the diagonal Elements of the matrix is shown & similarity transformation is done

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

$X^{-1}BX = B'$

$X^{-1}CX = C'$

$X^{-1}DX = D'$

Irreducible representation

Those representations which cannot be further reduced to representations of lower dimension are called irreducible representation.If it is not possible to find out similarity transformation matrix which will reduce the matrices of representation then the representation is said to be irreducible.All one dimensional representations are irreducible

Example - Matrices of transformation for z-coordinate of a Hydrogen atom in hydrogen molecule
Group - $D_{\infty h}$ group
Symmetry operation - E, C_{∞}, σ_v, σ_h, S_{∞}, C_2, i
The z-coordinate is unaffected by E, C_{∞}, σ_v operations
The equation for the transformation of z- coordinate of hydrogen atom by these operations are-

E.Z = 1Z	Ematrix = [1]
C_{∞}.Z = 1Z	$C_{\infty matrix}$ = [1]
σ_v.Z = 1Z	$\sigma_v$matrix = [1]

All the other operations of this group change the coordinate z of hydrogen atom into – z & the obtain equation for transformation are-

C_2.Z = - 1Z	$C_{2matrix}$ = [-1]
S_{∞}.Z = - 1Z	$S_{\infty matrix}$ = [-1]
σ_h.Z = - 1Z	$\sigma_h$matrix = [-1]
i.Z = - 1Z	imatrix = [-1]

The matrix representation thus obtained for z-coordinate of hydrogen atom in hydrogen molecule

	E	C_{∞}	σ_v	C_2	S_{∞}	σ_h	i
T	[1]	[1]	[1]	[-1]	[-1]	[-1]	[-1]

The representation T is irreducible since it is one dimensional.

The Great Orthogonality Theorem (GOT)

This theorem is concerned with the elements of matrices constituting irreducible representation of a point group. The properties of irreducible representations can be obtained from this theorem.

The GTO states:

$$\sum_{G} [\Gamma i(G)mn] [\Gamma j(G)m'n']^* = (h/\sqrt{lilj})\, \delta ij \delta mm' \delta nn'$$

Where,

1. *h*: Order of the group: the number of elements of the group.
2. i& j are two irreducible representation of the group.

3. ***li* & *lj*** are the dimensions of these two irreducible representation.
3. **Γ*i*:** *i*–th irreducible representation.
4. ***G***: Generic element of the group.It represents particular symmetry operation in the group
5. **Γ*i* (*G*)*mn*-** : Matrix element at the intersection of the *m*–th row with *n*–th column of the matrix representing *G* in the *i*–th irreducible representation.
6. **Γ*j* (*G*)*mn** -** The element in the m^{th}& n^{th} column of the matrix in the j^{th} irreducible representation.
7. **Γ*j*(*G*)*m′ n′* -** The complex conjugate of the element in the m^{th} row & n^{th} column of a matrix in the j^{th} irreducible representation.
8. ***δijδmm′ δnn′*-** Denotes Kornecker Delta symbol.The Kornecker Delta symbol ***δij*** has the meaning ***δij = 0* for i≠ j & *δij=1for i=j.***
It shows three cases
Case 1 - i = j, m = m′ **and *n = n′* simultaneously. Under such restrictions, equation** reduces to

$$\sum_G [\Gamma i(G)mn]\ [\Gamma i(G)m'n']^* = \sum_G ||\Gamma i(G)mn||^2 = h/li$$

this sum has as many terms as elements are in the group & the sum is over some matrix elements and their complex conjugate. In this case the numbers being multiplied by their complex conjugates can be considered as components of a vector, the result being the magnitude of the vector,hence the name given to the **orthogonality theorem**.

Case 2 - i≠j , [Γ*i*(*G*)*mn*] & [Γ*j*(*G*)*m′ n′*] represents two real elements in the m^{th} row & n^{th} column of a matrix for the operation G in the i&j representation

$$\sum_G [\Gamma i(G)mn]\ [\Gamma j(G)m'n']^* = (h/\sqrt{lilj})\ \delta ij = 0$$

It represents elements of corresponding matrices of different irreducible representation are orthogonal.

Case 3 - m≠ ***m′*** ***& n ≠ n′*** If **Γ*i* (*G*)*mn*** *is the* element in the m^{th} row & n^{th} column of the matrix for operation *G* in the i^{th} irreducible representation & **Γ*j*(*G*)*m′ n′*** *is the* element in the m'^{th} row & n'^{th} column of the matrix for operation *G* in the same representation then

$$\sum_G [\Gamma i(G)mn]\ [\Gamma j(G)m'n']^* = (h/\sqrt{li})\ \delta ij\delta mm'\ \delta nn' = 0$$

It represents elements of different set of matrices of same irreducible representation are orthogonal.

Importance of Orthogonality Theorem

It defines the properties of irreducible representation. By considering the three classes , 5 corollaries can be derived & these gives the 5 rules about the irreducible representation of a group & their character.

Rules for the irreducible representation

Again, let's state them now and prove them later. In the following discussion $\chi i(G)$ is the character (trace) of the matrix representing *G* in Γ*i*:
1.$\sum l2i = h$: The sum of the squares of the dimensions of the irreps equals The order of the group.
2.$\sum G\ |\chi i(G)|2 = h$: For a given irrep, the sum over all matrices of the squares of the magnitudes of the characters in the irrep equals the order of the group.
3.$\sum G\ \chi i(G)\chi j(G) = 0$: For any pair of irreps, the sum over all matrices of the products of the characters of the matrices representing the same element
Character tables
Sum of all the diagonal elements of a square matrix is known as character of matrix.

Symmetry operation	Character of matrix
Identity	3

Rotation	$2\cos\theta + 1$
Inversion	-3
Improper rotation	$2\cos\theta - 1$
Reflection	1

For each point group, a **character table** summarizes information on its symmetry operations and on its irreducible representations. As there are always equal numbers of irreducible representations and classes of symmetry operations, the tables are square.

The table itself consists of **characters** which represent how a particular irreducible representation transforms when a particular symmetry operation is applied. Any symmetry operation in a molecule's point group acting on the molecule itself will leave it unchanged. But for acting on a general entity, such as a vector or an orbital, this need not be the case. The Vector could change sign or direction, and the orbital could change type. For simple point groups, the values are either 1 or −1: 1 means that the sign or phase (of the vector or orbital) is unchanged by the symmetry operation (*symmetric*) and −1 denotes a sign change (*asymmetric*).

The representations are labeled according to a set of conventions:

- A, when rotation around the principal axis is symmetrical
- B, when rotation around the principal axis is asymmetrical
- E and T are doubly and triply degenerate representations, respectively when the point group has an inversion center
- the subscript g (German: *gerade* or even) signals no change in sign, and the subscript u (*ungerade* or uneven) a change in sign, with respect to inversion.with point groups $C_{\infty v}$
- $D_{\infty h}$ informs about how the Cartesian basis vectors, rotations about them, and quadratic functions of them transform by the symmetry operations of the group, by noting which irreducible representation transforms in t same way. These indications are conventionally on the right hand side of the tables.

This information is useful because chemically important orbitals (in particular *p* and *d* orbitals) have the same symmetries as these entities.

The character table for the C_{2v} symmetry point group is given below:

C_{2v}	E	C_2	$\sigma_v(xz)$	$\sigma_v'(yz)$		
A_1	1	1	1	1	Z	x^2, y^2, z^2
A_2	1	1	−1	−1	R_z	*Xy*
B_1	1	−1	1	−1	x, R_y	*Xz*
B_2	1	−1	−1	1	y, R_x	*Yz*

Example of water (H_2O) which has the C_{2v} symmetry . The $2p_x$ orbital of oxygen is oriented perpendicular to the plane of the molecule and switches sign with a C_2 and a $\sigma_v'(yz)$ operation, but remains unchanged with the other two operations (obviously, the character for the identity operation is always +1). This orbital's character set is thus {1, −1,1, −1}, corresponding to the B_1 irreducible representation. Similarly, the $2p_z$ orbital is seen to have the symmetry of the A_1 irreducible representation, $2p_y$ B_2, and the $3d_{xy}$ orbital A_2. These assignments and others are noted in the rightmost two columns of the table.

C_{3v}	E	$2C_3$	$3\sigma_v$		
A_1	1	1	1	z	$x^2 + y^2, z^2$
A_2	1	1	−1	R_z	
E	2	−1	0	$(x, y)(R_x, R_y)$	$(x^2 - y^2, xy)(xz, yz)$

The numbered regions contain the following contents.

1. The symbol used to represent the group in question (in this case C_{3v}).
2. The conjugacy classes, indicated by number and symbol, where the sum of the coefficients gives the group order of the group.
3. Mulliken symbols, one for each irreducible representation.
4. An array of the group characters of the irreducible representation of the group, with one column for each conjugacy class, and one row for each irreducible representation.
5. Combinations of the symbols x, y, z, R_x, R_y, and R_z, the first three of which represent the coordinates x, y, and z, and the last three of which stand for rotations about these axes. These are related to transformation properties and basis of representations of the group. All square and binary products of coordinates according to their transformation properties.

Due to the crystallographic restriction theorem, n is restricted to the values of 1, 2, 3, 4, or 6. It is important to note that the 'plane' in the definition of the rotation-reflection (alternating) axis of symmetry is **not necessarily** a mirror plane of the group in which the axis exists. Consider S_4, for example.Due to the crystallographic restriction theorem, $n = 1, 2, 3, 4$, or 6 in 2 or 3 dimension space.

Character Table & their uses

A finite group G has a finite number of conjugacy classes and a finite number of distinct irreducible representations. The group character of a group representation is constant on a conjugacy class. Hence, the values of the characters can be written as an array, known as a character table. Typically, the rows are given by the irreducible representations and the columns are given the conjugacy classes.A character table often contains enough information to identify a given abstract group and distinguish it from others. However, there exist nonisomorphic groups which nevertheless have the same character table, for example D_4 (the symmetry group of the square) and Q_8(the quaternion group).

For example, the symmetric group on three letters S_3 has three conjugacy classes, represented by the permutations $\{1, 2, 3\}$, $\{2, 1, 3\}$, and $\{2, 3, 1\}$. It also has three irreducible representations; two are one-dimensional and the third is two-dimensional:

1. The trivial representation $\phi_1(g)(\alpha) = \alpha$.
2. The alternating representation, given by the signature of the permutation, $\phi_2(g)(\alpha) = \operatorname{sgn}(g)\,\alpha$.
3. The standard representation on $V = \{(z_1, z_2, z_3) : \sum z_i = 0\}$ with

$$\phi_3(\{a, b, c\})(z_1, z_2, z_3) = (z_a, z_b, z_c).$$

The standard representation can be described on $\mathbb{C}^2$ via the matrices

$$\tilde{\phi}_3(\{2, 1, 3\}) = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

$$\tilde{\phi}_3(\{2, 3, 1\}) = \begin{bmatrix} 0 & -1 \\ 1 & -1 \end{bmatrix}.$$

and hence the group character of the first matrix is 0 and that of the second is -1. The group character of the identity is always the dimension of the vector space. The trace of the alternating representation is just the permutation symbol of the permutation. the character table for S_3 is shown below.

	1	2	3
S_3	e	(12)	(123)
Trivial	1	1	1
Alternating	1	-1	1
Standard	2	0	-1

N	1	2	3	4	6
C_n	C_1	C_2	C_3	C_4	C_6
C_{nv}	$C_{1v}=C_{1h}$	C_{2v}	C_{3v}	C_{4v}	C_{6v}
C_{nh}	C_{1h}	C_{2h}	C_{3h}	C_{4h}	C_{6h}
D_n	$D_1=C_2$	D_2	D_3	D_4	D_6
D_{nh}	$D_{1h}=C_{2v}$	D_{2h}	D_{3h}	D_{4h}	D_{6h}
D_{nd}	$D_{1d}=C_{2h}$	D_{2d}	D_{3d}	D_{4d}	D_{6d}
S_n	$S_1=C_{1h}$	S_2	$S_3=C_{3h}$	S_4	S_6

D_{4d} and D_{6d} are actually forbidden because they contain improper rotations with n=8 and 12 respectively. The 27 point groups in the table plus T, T_d, T_h, O and O_h constitute 32 crystallographic point groups

An irreducible representation of a group is a representation for which there exists no unitary transformation which will transform the representation matrix into block diagonal form. The irreducible representations have a number of remarkable properties, as formalized in the group orthogonality theorem

UNIT – 1

1. Which of the following is a symmetry element?
   a) Identity (E)
   b) Translation (T)
   c) Lattice point
   d) All of the above

Answer: a) Identity (E)

2. What is the symmetry element associated with a rotation by 360°/n about an axis?
   a) Inversion center
   b) Rotation axis (Cn)
   c) Reflection plane
   d) Identity (E)

Answer: b) Rotation axis (Cn)

3. What does a C2 rotation operation imply?
   a) 360° rotation
   b) 180° rotation
   c) 90° rotation
   d) 60° rotation

Answer: b) 180° rotation

4. What symmetry element corresponds to reflection through a plane?
   a) Mirror plane (σ)
   b) Inversion center (i)
   c) Rotation axis (Cn)
   d) Improper rotation (Sn)

Answer: a) Mirror plane (σ)

5. What is the notation for an improper rotation axis?
   a) Cn
   b) Sn
   c) i
   d) σ

Answer: b) Sn

6. A point group with no symmetry elements except identity is called:
   a) C∞
   b) C1
   c) S∞
   d) Cs

Answer: b) C1

7. Which symmetry element is associated with inversion through a point?
   a) σ
   b) Cn
   c) i
   d) E

Answer: c) i

8. The symmetry element that leaves all points unchanged is called:
   a) Identity (E)
   b) Inversion center (i)
   c) Rotation axis (Cn)
   d) Reflection plane (σ)

Answer: a) Identity (E)

9. What is the order of the symmetry element C4?
   a) 2
   b) 3
   c) 4
   d) 5

Answer: c) 4

10. The symmetry operation σh represents reflection through:
    a) A vertical plane
    b) A horizontal plane
    c) An inversion point
    d) A diagonal plane

Answer: b) A horizontal plane

11. Which of the following is an improper rotation?
    a) Cn
    b) i
    c) Sn
    d) E

Answer: c) Sn

12. Which point group contains only the identity operation?
    a) C∞v
    b) C1
    c) D2h
    d) S6

Answer: b) C1

13. What symmetry element is present in all molecules?
    a) σ
    b) C2
    c) E
    d) i

Answer: c) E

14. In water (H2O), what is the symmetry element present?
    a) C2
    b) C3
    c) C∞
    d) S4

Answer: a) C2

15. Which of the following operations is not a symmetry operation?
    a) Identity
    b) Reflection
    c) Inversion
    d) Translation

Answer: d) Translation

16. A reflection plane perpendicular to the principal axis is called:
    a) σh
    b) σv
    c) σd
    d) S2

Answer: a) σh

17. Which symmetry element involves rotation followed by reflection?
    a) Rotation axis
    b) Improper rotation (Sn)
    c) Mirror plane
    d) Inversion center

Answer: b) Improper rotation (Sn)

18. The molecule methane (CH4) belongs to which point group?
    a) D2d
    b) Td
    c) C3v
    d) C2h

Answer: b) Td

19. A point group that includes a C2 axis and two perpendicular C2 axes belongs to:
    a) C2v
    b) C3v
    c) D2
    d) D2h

Answer: c) D2

20. In a Cn point group, what symmetry operation is performed?
    a) Reflection
    b) Rotation
    c) Inversion
    d) Translation

Answer: b) Rotation

21. Which symmetry operation represents reflection through a vertical plane?
    a) σv
    b) σh
    c) σd
    d) Sn

Answer: a) σv

22. What is the symmetry element for a cube?
    a) C2
    b) C4
    c) C3
    d) All of the above

Answer: d) All of the above

23. How many mirror planes (σ) does benzene have?
    a) 3
    b) 6
    c) 5
    d) 4

Answer: b) 6

24. What is the principal axis of rotation for a trigonal bipyramidal molecule?
    a) C2
    b) C3
    c) C5
    d) C∞

Answer: c) C5

25. What is the symmetry element of a diatomic molecule?
    a) σ
    b) C∞
    c) C2
    d) i

Answer: b) C∞

26. Which of the following is a symmetry operation but not a symmetry element?
    a) Cn
    b) σ
    c) Rotation by 120°
    d) E

Answer: c) Rotation by 120°

27. Which symmetry element involves inversion at the origin?
    a) C2
    b) σv
    c) i
    d) Sn

Answer: c) i

28. Which of the following point groups contains an improper rotation axis?
    a) C1
    b) S6
    c) D2h
    d) C3v

Answer: b) S6

29. What is the symmetry element of a planar square molecule?
    a) C4
    b) C2
    c) σh
    d) All of the above

Answer: d) All of the above

30. Which of the following point groups belongs to linear molecules?
    a) C∞v
    b) Td
    c) D2h
    d) C2v

Answer: a) C∞v

31. What is the symmetry operation associated with S2?
    a) Reflection
    b) Rotation by 180°
    c) Rotation by 90° followed by reflection
    d) Identity

Answer: b) Rotation by 180°

32. A reflection plane that bisects angles between symmetry axes is called:
    a) σv
    b) σh
    c) σd
    d) S2

Answer: c) σd

33. The point group C2v contains how many symmetry elements?
    a) 2
    b) 4
    c) 6
    d) 8

Answer: b) 4

34. What is the principal symmetry element of a molecule with Td symmetry?
    a) C3
    b) C4
    c) C2
    d) i

Answer: a) C3

35. Which molecule belongs to the D6h point group?
    a) Methane (CH4)
    b) Benzene (C6H6)
    c) Water (H2O)
    d) Ammonia (NH3)

Answer: b) Benzene (C6H6)

36. What is the symmetry element of a tetrahedral molecule?
    a) C4
    b) C2
    c) C3
    d) σh

Answer: c) C3

37. In which point group does the ammonia (NH3) molecule belong?
    a) C3v
    b) C2v
    c) Td
    d) C∞v

Answer: a) C3v

38. How many symmetry elements does the identity (E) operation have?
    a) 1
    b) 2
    c) 0
    d) Infinite

Answer: a) 1

39. What is the symmetry element for a sphere?
    a) C2
    b) C∞
    c) i
    d) Td

Answer: b) C∞

40. What symmetry operation is associated with a Dn point group?
    a) Rotation only
    b) Reflection and inversion
    c) Rotation and perpendicular C2 axes
    d) Improper rotation

Answer: c) Rotation and perpendicular C2 axes

41. Which of the following is a symmetry operation?
   a) Reflection
   b) Rotation
   c) Inversion
   d) All of the above

Answer: d) All of the above

42. A C2 symmetry operation represents a rotation by:
   a) 360°
   b) 180°
   c) 90°
   d) 120°

Answer: b) 180°

43. The inversion operation (i) takes each point in a molecule through:
   a) The origin
   b) The reflection plane
   c) A rotational axis
   d) A perpendicular plane

Answer: a) The origin

44. What does the identity operation (E) do?
   a) Reflects the molecule
   b) Rotates the molecule
   c) Leaves the molecule unchanged
   d) Inverts the molecule

Answer: c) Leaves the molecule unchanged

45. A C3 symmetry operation is associated with which type of rotation?
   a) 120°
   b) 180°
   c) 90°
   d) 60°

Answer: a) 120°

46. A σv operation refers to a reflection through a:
   a) Horizontal plane
   b) Vertical plane
   c) Diagonal plane
   d) Inversion center

Answer: b) Vertical plane

47. The improper rotation Sn consists of:
   a) Only rotation
   b) Only reflection
   c) Rotation followed by reflection
   d) Reflection followed by inversion

Answer: c) Rotation followed by reflection

48. Which of the following operations is not a symmetry operation?
   a) Translation
   b) Reflection
   c) Rotation
   d) Inversion

Answer: a) Translation

49. In a C4 operation, the molecule is rotated by:
   a) 90°
   b) 120°
   c) 180°
   d) 60°

Answer: a) 90°

50. The symmetry operation that inverts all points through the center of the molecule is called:
   a) σh
   b) E
   c) C2
   d) Inversion (i)

Answer: d) Inversion (i)

51. Which operation combines rotation and reflection?
   a) Cn
   b) σ
   c) Sn
   d) i

Answer: c) Sn

52. The σh symmetry operation reflects a molecule through a:
   a) Horizontal plane
   b) Vertical plane
   c) Inversion center
   d) Diagonal plane

Answer: a) Horizontal plane

53. Which of the following is a rotation operation?
   a) Sn
   b) σ
   c) Cn
   d) E

Answer: c) Cn

54. A C∞ symmetry operation represents:
   a) Infinite inversion
   b) Infinite rotation
   c) Infinite reflection
   d) Identity operation

Answer: b) Infinite rotation

55. A symmetry operation that results in no change in the molecule is called:
   a) Reflection
   b) Identity
   c) Rotation
   d) Inversion

Answer: b) Identity

56. A symmetry operation that combines a 180° rotation followed by reflection is:
   a) C2
   b) S2
   c) σd
   d) i

Answer: b) S2

57. The symmetry operation σv in water (H2O) represents:
   a) A vertical plane reflection
   b) A horizontal plane reflection
   c) A 180° rotation
   d) An inversion

Answer: a) A vertical plane reflection

58. The Sn operation for S4 includes:
   a) 180° rotation and reflection
   b) 120° rotation and reflection
   c) 90° rotation and reflection
   d) 60° rotation and reflection

Answer: c) 90° rotation and reflection

59. Which of the following symmetry operations is always present in all molecules?
   a) σ
   b) E
   c) C2
   d) i

Answer: b) E

60. An S2 operation is equivalent to:
   a) A C2 operation
   b) A reflection
   c) An inversion
   d) A translation

Answer: c) An inversion

61. Which of the following is a combination of two symmetry operations?
 a) Cn
 b) Sn
 c) i
 d) E
Answer: b) Sn

62. The operation that takes each point of a molecule through a center of inversion is called:
 a) Reflection
 b) Identity
 c) Rotation
 d) Inversion
Answer: d) Inversion

63. How many degrees is the rotation in a C5 symmetry operation?
 a) 360°
 b) 90°
 c) 72°
 d) 60°
Answer: c) 72°

64. Which symmetry operation reflects a molecule through a diagonal plane?
 a) σh
 b) σv
 c) σd
 d) i
Answer: c) σd

65. The improper rotation Sn involves:
 a) Reflection only
 b) Inversion only
 c) Rotation and reflection
 d) Rotation and inversion
Answer: c) Rotation and reflection

66. A C3 operation rotates a molecule by:
 a) 180°
 b) 120°
 c) 90°
 d) 60°
Answer: b) 120°

67. Which symmetry operation involves rotating by 360°/n?
 a) Cn
 b) Sn
 c) σh
 d) E
Answer: a) Cn

68. A reflection through a plane that is parallel to the principal axis is called:
 a) σv
 b) σh
 c) σd
 d) C2
Answer: a) σv

69. The identity (E) operation is:
 a) A reflection
 b) A rotation
 c) A reflection and inversion
 d) The operation that leaves the molecule unchanged
Answer: d) The operation that leaves the molecule unchanged

70. Which symmetry operation leaves all points of a molecule unchanged?
 a) Cn
 b) Sn
 c) E
 d) i
Answer: c) E

71. What point group does a molecule with only the identity (E) operation belong to?
 a) C1
 b) Cs
 c) Ci
 d) C2v
Answer: a) C1

72. What point group does a linear molecule with a horizontal plane of symmetry belong to?
 a) D∞h
 b) C∞v
 c) C2v
 d) Td
Answer: a) D∞h

73. The ammonia (NH3) molecule belongs to which point group?
 a) C2v
 b) C3v
 c) Td
 d) D3h
Answer: b) C3v

74. A molecule with a C4 axis and four perpendicular C2 axes belongs to which point group?
 a) Td
 b) C4v
 c) D4h
 d) C3v
Answer: c) D4h

75. Which of the following point groups has only a single mirror plane and no other symmetry elements?
 a) C2v
 b) Cs
 c) C3v
 d) Td
Answer: b) Cs

76. Which point group includes a horizontal reflection plane (σh) but no vertical or diagonal planes?
 a) C3v
 b) Cs
 c) C2v
 d) C2h
Answer: d) C2h

77. The benzene molecule (C6H6) belongs to which point group?
 a) C2v
 b) Td
 c) D6h
 d) C3h
Answer: c) D6h

78. Which point group contains only the identity (E) and an inversion center (i)?
 a) C2v
 b) Cs
 c) Ci
 d) C1
Answer: c) Ci

79. Which point group corresponds to tetrahedral symmetry?
 a) Td
 b) Oh
 c) D3h
 d) D4h
Answer: a) Td

80. The water (H2O) molecule belongs to which point group?
 a) C2v
 b) Cs
 c) Td
 d) D3h

Answer: a) C2v

81. A molecule with a principal axis of rotation and no mirror planes or inversion centers belongs to which point group?
   a) Cn
   b) Cs
   c) Cnv
   d) Cnh

Answer: a) Cn

82. Which point group contains a C3 axis and three vertical mirror planes?
   a) C3h
   b) C3v
   c) C2v
   d) Td

Answer: b) C3v

83. A point group that contains a C2 axis and two perpendicular C2 axes is:
   a) C2v
   b) D2
   c) D3h
   d) Td

Answer: b) D2

84. Which point group contains a C2 axis and vertical mirror planes but no horizontal mirror planes?
   a) C2v
   b) C2h
   c) D3h
   d) S6

Answer: a) C2v

85. The molecule methane (CH_4) belongs to which point group?
   a) D2d
   b) Td
   c) C3v
   d) C2v

Answer: b) Td

86. Which point group is characterized by the presence of only a horizontal reflection plane?
   a) C2v
   b) Cs
   c) Ci
   d) Cnh

Answer: d) Cnh

87. A point group with a C5 axis and vertical mirror planes is:
   a) D5h
   b) C5v
   c) C5h
   d) Td

Answer: b) C5v

88. Which point group is associated with octahedral symmetry?
   a) D6h
   b) C4v
   c) Td
   d) Oh

Answer: d) Oh

89. The point group for a planar square molecule is:
   a) C4v
   b) D4h
   c) C2h
   d) C2v

Answer: b) D4h

90. Which point group does the diatomic hydrogen molecule (H_2) belong to?
   a) C2v
   b) D∞h
   c) C∞v
   d) D3h

Answer: c) C∞v

91. A molecule with a C3 axis and a horizontal mirror plane belongs to which point group?
   a) C3v
   b) C3h
   c) D3h
   d) D3d

Answer: b) C3h

92. Which point group contains a C2 axis, a σh, and two perpendicular C2 axes?
   a) D2h
   b) C2v
   c) D4h
   d) Td

Answer: a) D2h

93. Which point group does the allene (C_3H_4) molecule belong to?
   a) D2d
   b) Td
   c) C2v
   d) D3h

Answer: a) D2d

94. The point group for a trigonal planar molecule is:
   a) C3v
   b) D3h
   c) C2h
   d) Td

Answer: b) D3h

95. Which point group contains an improper rotation axis (Sn) and no other symmetry elements?
   a) Ci
   b) Cs
   c) Cn
   d) S6

Answer: d) S6

96. Which point group does the carbon dioxide (CO_2) molecule belong to?
   a) C∞v
   b) D∞h
   c) C2v
   d) Td

Answer: b) D∞h

97. Which point group contains two perpendicular C2 axes and no mirror planes or inversion center?
   a) D2
   b) D3h
   c) C2v
   d) D4h

Answer: a) D2

98. The point group containing only a horizontal mirror plane (σh) is:
   a) Cs
   b) Ci
   c) Cnh
   d) C2v

Answer: c) Cnh

99. What is the point group for an ethylene molecule (C_2H_4)?
   a) D2h
   b) C2v
   c) Td
   d) D∞h

Answer: a) D2h

100. A molecule with a C6 axis and six perpendicular C2 axes belongs to which point group?

a) D6h
b) C6v
c) C6h
d) D3h

Answer: a) D6h

101. Which point group has a C3 axis and three σv planes?
   a) C3v
   b) C3h
   c) D3h
   d) S6

Answer: a) C3v

102. Which point group is associated with a molecule with C∞ symmetry and no mirror planes?
   a) C∞v
   b) D∞h
   c) C2v
   d) S6

Answer: a) C∞v

103. What point group does the molecule SF6 belong to?
   a) Td
   b) D2h
   c) Oh
   d) C3v

Answer: c) Oh

104. A point group with C2 axis, vertical mirror planes, but no σh or inversion center belongs to:
   a) C2v
   b) D2h
   c) C2h
   d) Td

Answer: a) C2v

105. What point group does the square planar molecule XeF4 belong to?
   a) D2h
   b) Td
   c) C4v
   d) D4h

Answer: d) D4h

106. Which point group contains no reflection planes or inversion center but only a Cn axis?
   a) Cs
   b) Cnh
   c) Cn
   d) Ci

Answer: c) Cn

107. A molecule with Td symmetry has how many C3 axes?
   a) 1
   b) 3
   c) 4
   d) 6

Answer: c) 4

108. A molecule with octahedral symmetry (Oh) has how many mirror planes?
   a) 3
   b) 6
   c) 9
   d) 15

Answer: d) 15

109. Which point group does the PCl5 molecule belong to?
   a) Td
   b) D3h
   c) C4v
   d) C2v

Answer: b) D3h

110. Which point group contains a center of inversion but no mirror planes?
   a) C2v
   b) D2h
   c) Ci
   d) S6

Answer: c) Ci

111. What is a subgroup?
   a) A group that contains only one element
   b) A subset of a group that is itself a group
   c) A set of random elements
   d) A set of non-symmetric elements

Answer: b) A subset of a group that is itself a group

112. If H is a subgroup of G, then which of the following is true?
   a) H contains all the elements of G
   b) H is not closed under the group operation
   c) H must contain the identity element of G
   d) H contains no elements of G

Answer: c) H must contain the identity element of G

113. Which of the following is a necessary condition for H to be a subgroup of G?
   a) H is finite
   b) H is closed under the group operation
   c) H contains more elements than G
   d) H has no inverses

Answer: b) H is closed under the group operation

114. The set E, C2 in the group C2v is an example of:
   a) A trivial subgroup
   b) A non-trivial subgroup
   c) The whole group
   d) Not a subgroup

Answer: b) A non-trivial subgroup

115. Which of the following is a subgroup of the group C3v?
   a) C2v
   b) C2h
   c) C3
   d) Cs

Answer: d) Cs

116. A proper subgroup is defined as:
   a) A subgroup that contains the identity element only
   b) A subgroup that is equal to the original group
   c) A subgroup that is a proper subset of the group but not the entire group
   d) A subgroup that contains no identity element

Answer: c) A subgroup that is a proper subset of the group but not the entire group

117. In the group C4v, which of the following sets forms a subgroup?
   a) E, C4, C2, $C4^2$
   b) E, σv
   c) E, C2
   d) C4, σh

Answer: c) E, C2

118. A trivial subgroup is defined as:
   a) A subgroup that contains only the identity element
   b) A subgroup that contains all elements
   c) A subgroup that contains the identity and all symmetries
   d) A subgroup with no identity element

Answer: a) A subgroup that contains only the identity element

119. Which of the following point groups is a subgroup of Td?
   a) C3v
   b) D2h
   c) Oh
   d) D3h

Answer: a) C3v

120. If G is a group with order 6, which of the following is a possible order for a subgroup H of G?
   a) 7
   b) 8
   c) 3
   d) 9

Answer: c) 3

121. Which of the following point groups is a subgroup of D3h?
   a) D6h
   b) C3v
   c) C2v
   d) C4v

Answer: b) C3v

122. Which of the following is a subgroup of D4h?
   a) C4v
   b) C6h
   c) Td
   d) D3h

Answer: a) C4v

123. The identity element alone forms which kind of subgroup?
   a) Non-trivial subgroup
   b) Improper subgroup
   c) Cyclic subgroup
   d) Trivial subgroup

Answer: d) Trivial subgroup

124. Which of the following point groups is not a subgroup of Oh?
   a) C2v
   b) Td
   c) C3v
   d) C2h

Answer: d) C2h

125. Which of the following point groups is a subgroup of C4v?
   a) C3v
   b) C2v
   c) D4h
   d) C6v

Answer: b) C2v

126. If a subgroup H of a group G has only two elements, one of which is the identity, what kind of subgroup is H?
   a) Cyclic subgroup
   b) Improper subgroup
   c) Non-trivial subgroup
   d) Normal subgroup

Answer: a) Cyclic subgroup

127. In group theory, the concept of a coset is closely related to:
   a) Subgroups
   b) Symmetry elements
   c) Point groups
   d) Molecules

Answer: a) Subgroups

128. If a subgroup contains half the elements of a group, it is known as:
   a) A cyclic subgroup
   b) A Lagrange subgroup
   c) A normal subgroup
   d) An index-2 subgroup

Answer: d) An index-2 subgroup

129. Which point group is a subgroup of D2d?
   a) Td
   b) C2v
   c) Oh
   d) D6h

Answer: b) C2v

130. The alternating group A4 is a subgroup of which of the following groups?
   a) Oh
   b) D3h
   c) S4
   d) Td

Answer: c) S4

131. The order of a group is defined as:
   a) The number of operations in the group
   b) The number of elements in the group
   c) The highest power of an element in the group
   d) The number of subgroups in the group

Answer: b) The number of elements in the group

132. What is the order of a subgroup in relation to the order of the group?
   a) It must be a divisor of the group's order
   b) It must be greater than the group's order
   c) It can be any arbitrary number
   d) It is always equal to the order of the group

Answer: a) It must be a divisor of the group's order

133. Which theorem relates the order of a finite group to the order of its subgroups?
   a) Fermat's Little Theorem
   b) Lagrange's Theorem
   c) Abel's Theorem
   d) Cayley's Theorem

Answer: b) Lagrange's Theorem

134. If a group G has order 12, which of the following can be the order of a subgroup H of G?
   a) 7
   b) 6
   c) 13
   d) 9

Answer: b) 6

135. If H is a subgroup of G, and the order of G is 24, which of the following could be the order of H?
   a) 10
   b) 8
   c) 25
   d) 15

Answer: b) 8

136. According to Lagrange's theorem, if a group G has order 18, the possible orders of its subgroups are:
   a) 1, 2, 3, 6, 9, 18
   b) 1, 3, 6, 9, 18
   c) 1, 4, 9, 18
   d) 1, 2, 6, 12, 18

Answer: b) 1, 3, 6, 9, 18

137. If a group G has a prime order p, what are the possible orders of its subgroups?
   a) 1 and p
   b) Only p
   c) Any divisor of p
   d) 1, 2, and p

Answer: a) 1 and p

138. What is the order of a cyclic subgroup generated by an element a of order n in a group G?
   a) n
   b) n^2
   c) n/2
   d) 2n

Answer: a) n

139. If a group has order 15, what are the possible orders of its subgroups?
   a) 1, 3, 5, 15
   b) 1, 5, 10, 15

c) 1, 2, 3, 15
d) 1, 3, 7, 15

Answer: a) 1, 3, 5, 15

140. If H is a subgroup of a group G, and the order of G is 30, what are the possible orders of H?
a) 1, 2, 3, 5, 6, 10, 15, 30
b) 1, 3, 6, 9, 15, 30
c) 1, 4, 5, 10, 20
d) 1, 2, 5, 30

Answer: a) 1, 2, 3, 5, 6, 10, 15, 30

141. If a finite group G has a subgroup H, which of the following must be true?
a) The order of H divides the order of G
b) The order of G divides the order of H
c) The order of H must be greater than the order of G
d) The order of H is independent of G

Answer: a) The order of H divides the order of G

142. If G is a group of order 8, what are the possible orders of a cyclic subgroup of G?
a) 1 and 8
b) 1, 2, 4, 8
c) 1, 4, 8
d) 2, 4, 8

Answer: b) 1, 2, 4, 8

143. Which of the following statements about the order of a finite group and its subgroups is true?
a) A subgroup must have more elements than the group
b) A subgroup must have fewer elements than the group
c) The order of the subgroup is always a divisor of the group's order
d) The order of the subgroup is unrelated to the group's order

Answer: c) The order of the subgroup is always a divisor of the group's order

144. If the order of a group G is a prime number p, how many subgroups does G have?
a) Only 1
b) 2 (the identity subgroup and G itself)
c) p
d) p + 1

Answer: b) 2 (the identity subgroup and G itself)

145. If a group G has order 20, which of the following is not a possible order for a subgroup?
a) 2
b) 4
c) 5
d) 7

Answer: d) 7

146. If a group G has order 36, what are the possible orders of its subgroups?
a) 1, 2, 3, 4, 6, 9, 12, 18, 36
b) 1, 3, 6, 12, 36
c) 1, 4, 6, 18, 36
d) 1, 2, 4, 8, 16, 36

Answer: a) 1, 2, 3, 4, 6, 9, 12, 18, 36

147. In a group G of order 10, the order of any subgroup must be a divisor of:
a) 5
b) 10
c) 2
d) 20

Answer: b) 10

148. If a group G has order 24, which of the following could be the order of a subgroup?
a) 16
b) 24
c) 7
d) 9

Answer: b) 24

149. If the order of a group G is 40, what are the possible orders of its subgroups?
a) 1, 2, 4, 5, 8, 10, 20, 40
b) 1, 4, 8, 16, 40
c) 2, 5, 7, 40
d) 1, 3, 9, 40

Answer: a) 1, 2, 4, 5, 8, 10, 20, 40

150. If G is a group of order 21, which of the following can be the order of a subgroup?
a) 6
b) 7
c) 9
d) 14

Answer: b) 7

151. For any group (G), the size of the conjugacy class of an element (a) is equal to:
a) The order of (G)
b) The index of the centralizer of (a)
c) The order of (a)
d) The number of elements that commute with (a)

Answer: b) The index of the centralizer of (a)

152. In a symmetric group (Sn), which of the following determines the number of conjugacy classes?
a) The number of elements
b) The number of distinct cycle types
c) The number of transpositions
d) The number of permutations

Answer: b) The number of distinct cycle types

153. In a finite group, the number of conjugacy classes is equal to:
a) The number of subgroups
b) The number of irreducible characters
c) The number of elements of the group
d) The size of the group

Answer: b) The number of irreducible characters

154. In the cyclic group (C4), how many conjugacy classes are there?
a) 1
b) 2
c) 3
d) 4

Answer: a) 1

155. In a group (G) of order 12, which of the following is a possible number of conjugacy classes?
a) 4
b) 5
c) 6
d) 7

Answer: c) 6

156. The conjugacy class equation for a finite group (G) states that:
a) The sum of the sizes of conjugacy classes equals the order of the group
b) The sum of the sizes of the conjugacy classes equals the number of elements in the center
c) The sum of the sizes of the conjugacy classes equals the number of subgroups
d) The sum of the sizes of the conjugacy classes equals the number of normal subgroups

Answer: a) The sum of the sizes of conjugacy classes equals the order of the group

157. In a group (G) of order (n), if there are (k) conjugacy classes, the sum of the orders of the centralizers of representatives of these conjugacy classes is:
   a) (n)
   b) (n times k)
   c) (n div k)
   d) (n^2)

Answer: a) (n)

UNIT-2

1. What is a point group in the context of molecular symmetry?
   a) A group of all possible rotations
   b) A group that represents symmetry operations that leave a point fixed
   c) A set of all translation symmetries
   d) A group of all possible permutations

Answer: b) A group that represents symmetry operations that leave a point fixed

2. The point group (C2v) has how many symmetry elements?
   a) 2
   b) 3
   c) 4
   d) 6

Answer: c) 4

3. Which of the following point groups is characterized by having only one C_4 axis and no mirror planes?
   a) C4v
   b) D4h
   c) C4h
   d) C4

Answer: d) C4

4. The point group of a tetrahedral molecule like methane (CH_4) is:
   a) Td
   b) Oh
   c) C4v
   d) C3v

Answer: a) Td

5. The point group of a molecule with an octahedral geometry is:
   a) Td
   b) Oh
   c) C2v
   d) C3v

Answer: b) Oh

6. The point group of a molecule with one C_3 axis and three perpendicular mirror planes is:
   a) D3h
   b) C3v
   c) C2v
   d) D3d

Answer: a) D3h

7. In the point group (Dnh), what symmetry element is always present?
   a) A Cn axis
   b) A mirror plane perpendicular to the Cn axis
   c) A C2 axis
   d) An inversion center

Answer: b) A mirror plane perpendicular to the Cn axis

8. The point group of a linear molecule with no symmetry elements other than the identity and a rotation axis is:
   a) C∞v
   b) D∞h
   c) C2v
   d) Cs

Answer: a) C∞v

9. Which point group is associated with a molecule having a center of inversion but no mirror planes?
   a) C∞v
   b) D∞h
   c) S2n
   d) C2h

Answer: b) D∞h

10. The point group (C3v) contains:
   a) A C3 axis and three perpendicular C2 axes

b) A C3 axis and three mirror planes
c) A C3 axis and three perpendicular mirror planes
d) A C2 axis and a mirror plane

Answer: b) A C3 axis and three mirror planes

11. Which of the following point groups has a horizontal mirror plane and a C2 axis?
    a) D3h
    b) C2v
    c) C3v
    d) D4h

Answer: b) C2v

12. For a molecule in the (D3d) point group, the number of mirror planes is:
    a) 1
    b) 2
    c) 3
    d) 6

Answer: c) 3

13. The point group of a molecule with a single C_2 axis and two perpendicular mirror planes is:
    a) C2v
    b) D2h
    c) C∞v
    d) D∞h

Answer: b) D2h

14. A molecule with (D4h) point group symmetry has:
    a) One C4 axis and two perpendicular C2 axes
    b) One C4 axis, four C2 axes, and mirror planes
    c) Four C2 axes and a horizontal mirror plane
    d) No symmetry elements

Answer: b) One C4 axis, four C2 axes, and mirror planes

15. The point group of a molecule with two perpendicular C3 axes and mirror planes is:
    a) D3h
    b) C3v
    c) D6h
    d) D3d

Answer: d) D3d

16. In the point group (C2h), the symmetry elements include:
    a) One C2 axis and two mirror planes
    b) One C2 axis and an inversion center
    c) Two C2 axes and a horizontal mirror plane
    d) A C2 axis and a vertical mirror plane

Answer: b) One C2 axis and an inversion center

17. Which point group has a single C2 axis and no other symmetry elements?
    a) C2v
    b) C2
    c) Cs
    d) C∞v

Answer: b) C2

18. The point group of a molecule with (D6h) symmetry includes:
    a) One C6 axis, three C2 axes, and horizontal mirror planes
    b) One C6 axis and one C2 axis
    c) One C6 axis and vertical mirror planes
    d) One C6 axis and perpendicular mirror planes

Answer: a) One C6 axis, three C2 axes, and horizontal mirror planes

19. Which of the following point groups includes an inversion center?
    a) C2v
    b) C3v
    c) D2h
    d) D∞h

Answer: c) D2h

20. In the (Td) point group, the symmetry elements include:
    a) Four C3 axes and mirror planes
    b) Three C2 axes and mirror planes
    c) Three C2 axes and a center of inversion
    d) Four C3 axes and inversion center

Answer: a) Four C3 axes and mirror planes

21. The point group of a molecule with a mirror plane and no other symmetry elements is:
    a) Cs
    b) C2v
    c) D2h
    d) C∞v

Answer: a) Cs

22. The point group (Sn) is characterized by:
    a) A Cn axis and n mirror planes
    b) A Cn axis and n perpendicular C2 axes
    c) An n-fold improper rotation axis
    d) A single mirror plane

Answer: c) An n-fold improper rotation axis

23. In which point group does a molecule have a C3 axis and a horizontal mirror plane, but no vertical mirror planes?
    a) D3h
    b) C3v
    c) C2v
    d) D3d

Answer: a) D3h

24. The point group of a molecule with C5 symmetry is:
    a) C5v
    b) D5h
    c) C5
    d) D5

Answer: c) C5

25. The point group of a molecule with three perpendicular mirror planes and a center of inversion is:
    a) D3h
    b) D2h
    c) C2h
    d) Oh

Answer: b) D2h

26. For a molecule in the (D5h) point group, which symmetry elements are present?
    a) One C5 axis, horizontal mirror planes, and five perpendicular C2 axes
    b) One C5 axis, a horizontal mirror plane, and five perpendicular C2 axes
    c) One C5 axis and five mirror planes
    d) One C5 axis and one mirror plane

Answer: a) One C5 axis, horizontal mirror planes, and five perpendicular C2 axes

27. The point group of a molecule with a C2 axis and a vertical mirror plane but no horizontal mirror plane is:
    a) C2v
    b) D2h
    c) C2
    d) Cs

Answer: a) C2v

28. In the (Oh) point group, how many C4 axes are present?
    a) 1
    b) 2
    c) 3
    d) 4

Answer: d) 4

29. A molecule with a single C4 axis and four perpendicular C2 axes belongs to which point group?
    a) C4v
    b) D4h

c) C4h
d) Td

Answer: b) D4h

30. The point group of a molecule with a single C3 axis and no other symmetry elements is:
a) C3
b) D3
c) C3v
d) C2v

Answer: a) C3

31. The Schoenflies symbol (C2v) represents a point group with:
a) A single C2 axis and two perpendicular mirror planes
b) A single C2 axis and one mirror plane
c) A C2 axis and a C3 axis
d) A C2 axis and a C4 axis

Answer: a) A single C2 axis and two perpendicular mirror planes

32. What is the Schoenflies symbol for a point group with one C3 axis and three vertical mirror planes?
a) C3v
b) D3h
c) C3h
d) D3

Answer: a) C3v

33. The Schoenflies symbol (D2h) denotes a point group with:
a) Two C2 axes perpendicular to each other and a horizontal mirror plane
b) A single C2 axis and an inversion center
c) A C2 axis and two vertical mirror planes
d) Three C2 axes and a center of inversion

Answer: a) Two C2 axes perpendicular to each other and a horizontal mirror plane

34. The point group (Td) is characterized by:
a) Four C3 axes and mirror planes
b) A single C4 axis and perpendicular C2 axes
c) Four C3 axes and an inversion center
d) A C2 axis and mirror planes

Answer: a) Four C3 axes and mirror planes

35. Which Schoenflies symbol represents a point group with only a single C2 axis and no mirror planes?
a) C2
b) C2v
c) C2h
d) Cs

Answer: a) C2

36. The Schoenflies symbol (D4h) corresponds to a point group with:
a) One C4 axis, two perpendicular C2 axes, and horizontal mirror planes
b) One C4 axis and one mirror plane
c) Four C2 axes and vertical mirror planes
d) A C2 axis and four mirror planes

Answer: a) One C4 axis, two perpendicular C2 axes, and horizontal mirror planes

37. What is the Schoenflies symbol for a point group with an infinite Cn axis and vertical mirror planes?
a) C∞v
b) D∞h
c) Cn
d) Dn

Answer: a) C∞v

38. The point group (C4v) has:
a) A single C4 axis and four vertical mirror planes
b) One C4 axis and two perpendicular mirror planes
c) Four C2 axes and one horizontal mirror plane
d) One C4 axis and an inversion center

Answer: a) A single C4 axis and four vertical mirror planes

39. The Schoenflies symbol (C3h) represents a point group with:
a) A single C3 axis and a horizontal mirror plane
b) A single C3 axis and three perpendicular C2 axes
c) Three C2 axes and a vertical mirror plane
d) A single C3 axis and no mirror planes

Answer: a) A single C3 axis and a horizontal mirror plane

40. Which Schoenflies symbol represents a point group with a center of inversion and no mirror planes?
a) D∞h
b) C∞v
c) C2h
d) C2v

Answer: c) C2h

41. The Schoenflies symbol (D6h) denotes a point group with:
a) One C6 axis, three C2 axes, and horizontal mirror planes
b) One C6 axis and six perpendicular C2 axes
c) One C6 axis and no mirror planes
d) Three C2 axes and an inversion center

Answer: a) One C6 axis, three C2 axes, and horizontal mirror planes

42. The point group (D3h) includes:
a) One C3 axis, three perpendicular mirror planes, and a horizontal mirror plane
b) One C3 axis, three mirror planes, and one C2 axis
c) A C2 axis and three vertical mirror planes
d) One C3 axis and three perpendicular C2 axes

Answer: a) One C3 axis, three perpendicular mirror planes, and a horizontal mirror plane

43. In the Schoenflies symbol (D2d), what symmetry elements are present?
a) Two C2 axes perpendicular to each other and two diagonal mirror planes
b) Two C2 axes perpendicular to each other and a horizontal mirror plane
c) One C2 axis and three perpendicular C2 axes
d) A single C2 axis and an inversion center

Answer: a) Two C2 axes perpendicular to each other and two diagonal mirror planes

44. The point group (Oh) has:
a) Four C4 axes and horizontal mirror planes
b) Four C2 axes and vertical mirror planes
c) Three C2 axes and horizontal mirror planes
d) One C2 axis and one horizontal mirror plane

Answer: a) Four C4 axes and horizontal mirror planes

45. The Schoenflies symbol (S4) represents a point group with:
a) An S4 axis and four mirror planes
b) A C4 axis and four perpendicular mirror planes
c) A single S4 axis and a horizontal mirror plane
d) An S4 axis and perpendicular C2 axes

Answer: a) An S4 axis and four mirror planes

46. In the Schoenflies notation, the symbol (C∞v) describes a point group with:
a) An infinite Cn axis and vertical mirror planes
b) An infinite number of perpendicular mirror planes
c) A single C∞ axis and a horizontal mirror plane
d) A single C∞ axis and no mirror planes

Answer: a) An infinite Cn axis and vertical mirror planes

47. The point group (C2h) includes:
a) A single C2 axis and a horizontal mirror plane
b) A single C2 axis and two vertical mirror planes
c) Two C2 axes and horizontal mirror planes
d) A C2 axis and vertical mirror planes

Answer: a) A single C2 axis and a horizontal mirror plane

48. The Schoenflies symbol (C4h) corresponds to a point group with:
   a) One C4 axis and a horizontal mirror plane
   b) Two C4 axes and mirror planes
   c) Four C2 axes and vertical mirror planes
   d) One C4 axis and vertical mirror planes

Answer: a) One C4 axis and a horizontal mirror plane

49. The point group (D3d) is characterized by:
   a) Three C2 axes perpendicular to each other and diagonal mirror planes
   b) Three C2 axes and horizontal mirror planes
   c) One C3 axis and three perpendicular mirror planes
   d) One C3 axis and diagonal mirror planes

Answer: a) Three C2 axes perpendicular to each other and diagonal mirror planes

50. Which Schoenflies symbol denotes a point group with only the identity operation and no other symmetry elements?
   a) C1
   b) Cs
   c) C2
   d) D2h

Answer: a) C1

51. The Schoenflies symbol (D4) represents a point group with:
   a) A single C4 axis and four C2 axes
   b) Two C4 axes and horizontal mirror planes
   c) A single C4 axis and four perpendicular C2 axes
   d) Four C2 axes and no mirror planes

Answer: c) A single C4 axis and four perpendicular C2 axes

52. The point group (S6) is characterized by:
   a) An S6 axis and six mirror planes
   b) An S6 axis and one C6 axis
   c) A C6 axis and six perpendicular mirror planes
   d) An S6 axis and a horizontal mirror plane

Answer: a) An S6 axis and six mirror planes

53. The Schoenflies symbol (C3h) denotes a point group with:
   a) A single C3 axis and a horizontal mirror plane
   b) A single C3 axis and three vertical mirror planes
   c) Three C2 axes and a horizontal mirror plane
   d) Three perpendicular C2 axes and a horizontal mirror plane

Answer: a) A single C3 axis and a horizontal mirror plane

54. The point group (C2v) includes:
   a) One C2 axis and two perpendicular mirror planes
   b) One C2 axis and a horizontal mirror plane
   c) Two C2 axes and vertical mirror planes
   d) One C2 axis and no mirror planes

Answer: a) One C2 axis and two perpendicular mirror planes

55. The Schoenflies symbol (D6h) corresponds to a point group with:
   a) One C6 axis, perpendicular C2 axes, and horizontal mirror planes
   b) One C6 axis and one horizontal mirror plane
   c) Three C2 axes and vertical mirror planes
   d) Six C2 axes and no mirror planes

Answer: a) One C6 axis, perpendicular C2 axes, and horizontal mirror planes

56. Which point group is represented by the Schoenflies symbol (D4d)?
   a) A single C4 axis and two perpendicular C2 axes with diagonal mirror planes
   b) Four C2 axes and horizontal mirror planes
   c) One C4 axis and four perpendicular C2 axes
   d) One C4 axis and vertical mirror planes

Answer: a) A single C4 axis and two perpendicular C2 axes with diagonal mirror planes

57. The Schoenflies symbol (C5v) denotes a point group with:
   a) A single C5 axis and five vertical mirror planes
   b) A single C5 axis and one mirror plane
   c) Five C2 axes and a horizontal mirror plane
   d) A single C5 axis and five perpendicular C2 axes

Answer: a) A single C5 axis and five vertical mirror planes

58. The point group (D2) includes:
   a) Two perpendicular C2 axes and no mirror planes
   b) Two C2 axes and a horizontal mirror plane
   c) A single C2 axis and two vertical mirror planes
   d) Two C2 axes and diagonal mirror planes

Answer: a) Two perpendicular C2 axes and no mirror planes

59. The Schoenflies symbol (S4) represents a point group with:
   a) An S4 axis and four mirror planes
   b) A single S4 axis and vertical mirror planes
   c) An S4 axis and horizontal mirror planes
   d) A single S4 axis and no mirror planes

Answer: a) An S4 axis and four mirror planes

60. The Schoenflies symbol (D2d) includes:
   a) Two C2 axes and two diagonal mirror planes
   b) Two C2 axes and a horizontal mirror plane
   c) One C2 axis and two vertical mirror planes
   d) Three C2 axes and diagonal mirror planes

Answer: a) Two C2 axes and two diagonal mirror planes

61. The number of irreducible representations of the point group (Cn) is:
   a) (n)
   b) (n+1)
   c) (n-1)
   d) (2n)

Answer: a) (n)

62. In the (C2v) point group, how many irreducible representations are there?
   a) 2
   b) 3
   c) 4
   d) 5

Answer: b) 3

63. The point group (C4v) has how many 2-dimensional irreducible representations?
   a) 1
   b) 2
   c) 3
   d) 4

Answer: b) 2

64. For the (D3h) point group, how many irreducible representations are there?
   a) 4
   b) 6
   c) 7
   d) 5

Answer: b) 6

65. The character table for the (C2h) point group includes how many different irreducible representations?
   a) 2
   b) 3
   c) 4
   d) 5

Answer: c) 4

66. The point group (D4h) has how many 4-dimensional irreducible representations?
   a) 1
   b) 2
   c) 3
   d) 4

Answer: a) 1

67. In the point group (C6v), how many irreducible representations are there?
- a) 6
- b) 7
- c) 8
- d) 9

Answer: b) 7

68. The point group (D2d) has how many 2-dimensional irreducible representations?
- a) 2
- b) 3
- c) 4
- d) 5

Answer: a) 2

69. For the point group (D6h), the number of irreducible representations is:
- a) 5
- b) 6
- c) 7
- d) 8

Answer: d) 8

70. The character table for (C2v) includes which of the following irreducible representations?
- a) A1, A2, B1, B2
- b) A, B, E
- c) A1g, A2g, Eg
- d) E, T2

Answer: a) A1, A2, B1, B2

71. In the (C3v) point group, the number of irreducible representations is:
- a) 2
- b) 3
- c) 4
- d) 5

Answer: b) 3

72. The character table of (D3h) includes how many 3-dimensional irreducible representations?
- a) 1
- b) 2
- c) 3
- d) 4

Answer: c) 1

73. For the (C4h) point group, which of the following is a valid irreducible representation?
- a) A1g
- b) B1g
- c) Eg
- d) T2g

Answer: a) A1g

74. The point group (D2h) has how many irreducible representations in total?
- a) 6
- b) 8
- c) 4
- d) 5

Answer: b) 8

75. In the point group (C2v), the irreducible representation (B1) is characterized by:
- a) A C2 axis and a mirror plane
- b) A C2 axis and perpendicular mirror planes
- c) A horizontal mirror plane
- d) A vertical mirror plane

Answer: d) A vertical mirror plane

76. The number of irreducible representations for the (D4h) point group is:
- a) 6
- b) 8
- c) 10
- d) 12

Answer: b) 8

77. Which point group has the irreducible representation (A1g)?
- a) (C2v)
- b) (D4h)
- c) (C3v)
- d) (D3h)

Answer: b) (D4h)

78. The point group (D5h) includes how many 2-dimensional irreducible representations?
- a) 1
- b) 2
- c) 3
- d) 4

Answer: b) 2

79. In (Cnh) point groups, the number of 1-dimensional irreducible representations is:
- a) 1
- b) 2
- c) 3
- d) 4

Answer: b) 2

80. For the point group (C6v), the number of 2-dimensional irreducible representations is:
- a) 1
- b) 2
- c) 3
- d) 4

Answer: b) 2

81. The character table for (D3h) includes which of the following irreducible representations?
- a) A1g, A2g, B1g, B2g
- b) A1, A2, E
- c) A1, A2, E1, E2
- d) A1g, A2g, Eg, T1u

Answer: c) A1, A2, E1, E2

82. In the (C2h) point group, which of the following is a 1-dimensional irreducible representation?
- a) Ag
- b) Bg
- c) Au
- d) Bu

Answer: a) Ag

83. For the (D6h) point group, which irreducible representation is 4-dimensional?
- a) A1g
- b) Eg
- c) T1u
- d) T2g

Answer: d) T2g

84. In the point group (C2v), which of the following is a 2-dimensional irreducible representation?
- a) A1
- b) B2
- c) B1
- d) E

Answer: d) E

85. The number of 1-dimensional irreducible representations in the (D4h) point group is:
- a) 2
- b) 3
- c) 4
- d) 5

Answer: c) 4

86. The point group (C3v) has which type of irreducible representations?
   a) A1, A2, E
   b) A1g, A2g, Eg
   c) A1g, A2g, T1u
   d) Ag, Bg, Eg

Answer: a) A1, A2, E

87. For the point group (D4h), which representation is known for having the character '1' for all symmetry operations?
   a) A1g
   b) B1g
   c) Eg
   d) T2g

Answer: a) A1g

88. The point group (D2h) includes which irreducible representation?
   a) A1g, A2g, B1g, B2g
   b) A1g, A2g, Eg
   c) A1, A2, B1, B2
   d) A1, A2, E

Answer: a) A1g, A2g, B1g, B2g

89. The number of irreducible representations for the (C4v) point group is:
   a) 3
   b) 4
   c) 5
   d) 6

Answer: b) 4

90. In the point group (C3v), the irreducible representation (A2) is characterized by:
   a) Being symmetric with respect to all mirror planes
   b) Changing sign under a C3 rotation
   c) Being antisymmetric with respect to all mirror planes
   d) Having no change under C3 rotation

Answer: b) Changing sign under a C3 rotation

91. The character table for the (D5h) point group includes how many 3-dimensional irreducible representations?
   a) 1
   b) 2
   c) 3
   d) 4

Answer: a) 1

92. In the point group (C2v), which representation is a 2-dimensional representation?
   a) A1
   b) B1
   c) B2
   d) E

Answer: d) E

93. For the (D4d) point group, which irreducible representation has the character '0' for all symmetry operations?
   a) A1
   b) E
   c) B1
   d) B2

Answer: b) E

94. The point group (Cnh) has how many 2-dimensional irreducible representations?
   a) 1
   b) 2
   c) 3
   d) 4

Answer: b) 2

95. In the point group (D6h), which irreducible representation corresponds to a 2-dimensional matrix representation?
   a) Eg
   b) T1g
   c) T2g
   d) A1g

Answer: a) Eg

96. The character table for the (D4h) point group includes which of the following irreducible representations?
   a) A1g, A2g, Eg, T1g, T2g
   b) A1, A2, B1, B2, E
   c) Ag, Bg, Eg, T1u
   d) A1g, A2g, B1g, B2g

Answer: d) A1g, A2g, B1g, B2g

97. The number of 1-dimensional irreducible representations in the (D3h) point group is:
   a) 1
   b) 2
   c) 3
   d) 4

Answer: b) 2

98. The point group (C2v) includes how many 1-dimensional irreducible representations?
   a) 1
   b) 2
   c) 3
   d) 4

Answer: b) 2

99. In the (D2h) point group, which of the following is a 2-dimensional irreducible representation?
   a) B1g
   b) B2g
   c) Eg
   d) A1g

Answer: c) Eg

100. For the (D6h) point group, which representation is 3-dimensional?
   a) A1g
   b) T1g
   c) Eg
   d) B2g

Answer: b) T1g

101. The character of a representation is defined as:
   a) The trace of the matrix representing the symmetry operation
   b) The determinant of the matrix representing the symmetry operation
   c) The eigenvalue of the matrix representing the symmetry operation
   d) The norm of the matrix representing the symmetry operation

Answer: a) The trace of the matrix representing the symmetry operation

102. In the context of group theory, the character of a representation is used to:
   a) Determine the number of symmetry operations
   b) Identify the symmetry elements
   c) Classify the irreducible representations
   d) Compute the symmetry of a molecule

Answer: c) Classify the irreducible representations

103. The character of a representation of the identity element of a group is always:
   a) 0
   b) 1
   c) Equal to the dimension of the representation
   d) Negative

Answer: c) Equal to the dimension of the representation

104. The character of a representation for a symmetry operation that leaves the molecule unchanged is:
   a) 0
   b) Equal to the dimension of the representation
   c) 1
   d) -1

Answer: b) Equal to the dimension of the representation

105. For a 2-dimensional representation, the character of a rotation by 180° (C2) is:
   a) 2
   b) 0
   c) 1
   d) -2

Answer: a) 2

106. The character of a representation for an inversion operation (i) is:
   a) The trace of the matrix representing the inversion
   b) Equal to the dimension of the representation
   c) Always 0
   d) The eigenvalue of the matrix representing the inversion

Answer: a) The trace of the matrix representing the inversion

107. In the character table, the character for a C3 rotation in a 3-dimensional representation is:
   a) 1
   b) 0
   c) 2
   d) -1

Answer: a) 1

108. The sum of the squares of the characters of a representation over all symmetry operations of a group is equal to:
   a) The number of symmetry operations
   b) The product of the number of irreducible representations
   c) The order of the group
   d) The dimension of the group

Answer: c) The order of the group

109. For a 1-dimensional representation, the character of any symmetry operation is:
   a) Always 0
   b) Always 1
   c) Equal to the dimension of the operation
   d) Varies with the operation

Answer: b) Always 1

110. In a character table, the character of a reflection operation in the xy-plane for a 2-dimensional representation is typically:
   a) 2
   b) 1
   c) 0
   d) -1

Answer: c) 0

111. The character of a representation for a C4 rotation in a 4-dimensional representation is:
   a) 4
   b) 0
   c) 1
   d) -1

Answer: a) 4

112. The character of a reflection in the xz-plane in a 3-dimensional representation is:
   a) 1
   b) 0
   c) -1
   d) 2

Answer: b) 0

113. The character of a representation for a symmetry operation is used to determine:
   a) The bond angles
   b) The molecular orbitals
   c) The symmetry of the molecule
   d) The vibrational frequencies

Answer: c) The symmetry of the molecule

114. For a 3-dimensional representation, the character of a C2 rotation is:
   a) 0
   b) 1
   c) 2
   d) 3

Answer: a) 0

115. The character of a representation for an operation that does not change the molecule's symmetry is:
   a) The trace of the matrix representing the operation
   b) The determinant of the matrix representing the operation
   c) Always 0
   d) The eigenvalue of the matrix representing the operation

Answer: a) The trace of the matrix representing the operation

116. The character of a representation for a C6 rotation in a 6-dimensional representation is:
   a) 1
   b) 0
   c) 6
   d) -1

Answer: a) 1

117. The character of the identity element of a group in any representation is equal to:
   a) The dimension of the representation
   b) 0
   c) 1
   d) The number of irreducible representations

Answer: a) The dimension of the representation

118. The character of a representation for a reflection operation in the yz-plane is:
   a) 1
   b) 0
   c) -1
   d) 2

Answer: b) 0

119. For a 4-dimensional representation, the character of a C4 rotation is:
   a) 1
   b) 0
   c) 4
   d) 2

Answer: c) 4

120. The character of a representation for a mirror plane operation in a 2-dimensional representation is:
   a) 0
   b) 1
   c) 2
   d) -1

Answer: a) 0

121. In the character table for (D2h), the character of a C2 rotation is:
   a) Always 0
   b) Always 1
   c) Varies with the representation
   d) Always -1

Answer: c) Varies with the representation

122. The character of a reflection operation in the xy-plane for a 1-dimensional representation is:
   a) 1
   b) 0
   c) -1
   d) 2

Answer: c) -1

123. In the character table for (C3v), the character for a C3 rotation is:
   a) 1
   b) 0
   c) 2
   d) -1

Answer: a) 1

124. For a 2-dimensional representation, the character of a C3 rotation is:
   a) 0
   b) 1
   c) 2
   d) -1

Answer: a) 0

125. The character of a representation for a C2 rotation in a 1-dimensional representation is:
   a) Always 1
   b) Always 0
   c) Varies with the operation
   d) Always -1

Answer: a) Always 1

126. The character of a reflection operation in a 3-dimensional representation typically has:
   a) The same value for all reflections
   b) The value 0
   c) The value 1
   d) The value -1

Answer: b) The value 0

127. The character of a C2 rotation in the (D4h) point group is:
   a) 0
   b) 2
   c) 4
   d) -2

Answer: b) 2

128. The sum of the characters for each symmetry operation in a given representation is:
   a) Always 0
   b) The order of the group
   c) The dimension of the representation
   d) The trace of the matrix

Answer: b) The order of the group

129. The character of the identity element in a 2-dimensional representation is:
   a) 0
   b) 1
   c) 2
   d) -1

Answer: c) 2

130. The character of a C4 rotation in a 3-dimensional representation is:
   a) 0
   b) 1
   c) 2
   d) -1

Answer: a) 0

UNIT - 3

1. A representation that cannot be decomposed into smaller representations is called:
   a) Reducible
   b) Irreducible
   c) Trivial
   d) Symmetric

Answer: b) Irreducible

2. A representation that can be expressed as a direct sum of smaller representations is:
   a) Irreducible
   b) Reducible
   c) Trivial
   d) Regular

Answer: b) Reducible

3. The process of finding the irreducible components of a reducible representation is known as:
   a) Characterization
   b) Reduction
   c) Diagonalization
   d) Symmetrization

Answer: b) Reduction

4. In group theory, the character of a reducible representation is:
   a) Always zero
   b) The sum of the characters of its irreducible components
   c) The same as the character of its largest component
   d) Not well-defined

Answer: b) The sum of the characters of its irreducible components

5. A matrix representation is said to be reducible if:
   a) It has only one non-zero eigenvalue
   b) It can be brought to block diagonal form by a similarity transformation
   c) It is diagonalizable
   d) It has all distinct eigenvalues

Answer: b) It can be brought to block diagonal form by a similarity transformation

6. The dimension of an irreducible representation is always:
   a) 1
   b) Equal to or less than the dimension of the reducible representation
   c) Greater than the dimension of the reducible representation
   d) A multiple of the dimension of the reducible representation

Answer: b) Equal to or less than the dimension of the reducible representation

7. The process of determining whether a representation is irreducible or not involves:
   a) Calculating the eigenvalues
   b) Finding the character table
   c) Performing similarity transformations
   d) Applying group theory operations

Answer: c) Performing similarity transformations

8. If a representation of a group has only one irreducible component, it is:
   a) Trivial
   b) Reducible
   c) Irreducible
   d) Non-decomposable

Answer: c) Irreducible

9. The character of a reducible representation is the sum of:
   a) The eigenvalues
   b) The characters of its irreducible components
   c) The dimensions of the irreducible components
   d) The diagonal elements of the matrix

Answer: b) The characters of its irreducible components

10. The reduction of a reducible representation is useful for:
   a) Simplifying matrix calculations
   b) Identifying the symmetry of a molecule
   c) Determining the molecular orbitals
   d) Finding the irreducible components

Answer: d) Finding the irreducible components

11. In the context of group theory, the term "reduction" refers to:
   a) Increasing the size of a representation
   b) Decomposing a reducible representation into irreducible components
   c) Simplifying the group structure
   d) Transforming a representation to a higher dimension

Answer: b) Decomposing a reducible representation into irreducible components

12. The irreducible representations of a group can be:
   a) Determined directly from the reducible representation
   b) Found using the character table
   c) Equal to the number of symmetry operations
   d) Found by trial and error

Answer: b) Found using the character table

13. The dimension of a reducible representation is:
   a) Always greater than that of any of its irreducible components
   b) Equal to the sum of the dimensions of its irreducible components
   c) Always less than the dimension of its largest irreducible component
   d) Unrelated to the dimensions of its irreducible components

Answer: b) Equal to the sum of the dimensions of its irreducible components

14. If a reducible representation is decomposed into irreducible components, the resulting irreducible representations are:
   a) Always the same size
   b) Only 1-dimensional
   c) Unique to the group
   d) May vary in size and dimension

Answer: d) May vary in size and dimension

15. To find the number of times an irreducible representation appears in a reducible representation, one can use:
   a) The determinant method
   b) The trace method
   c) The orthogonality theorem
   d) The eigenvalue method

Answer: c) The orthogonality theorem

16. The orthogonality theorem states that:
   a) The characters of different irreducible representations are orthogonal
   b) The characters of the same irreducible representation are orthogonal
   c) The eigenvectors of different matrices are orthogonal
   d) The dimensions of different irreducible representations are orthogonal

Answer: a) The characters of different irreducible representations are orthogonal

17. For a reducible representation, the trace of the matrix for a symmetry operation is:
   a) The sum of the traces of its irreducible components
   b) The product of the traces of its irreducible components
   c) Always zero
   d) Not directly related to the irreducible components

Answer: a) The sum of the traces of its irreducible components

18. In a character table, the number of irreducible representations is equal to:
   a) The number of symmetry elements in the group
   b) The order of the group
   c) The number of conjugacy classes in the group
   d) The dimension of the reducible representation

Answer: c) The number of conjugacy classes in the group

19. The dimensions of the irreducible representations of a group always sum up to:
   a) The number of symmetry operations
   b) The order of the group
   c) The number of irreducible representations
   d) The dimension of the reducible representation

Answer: b) The order of the group

20. A matrix representation is said to be irreducible if:
   a) It cannot be diagonalized
   b) It cannot be decomposed into smaller representations
   c) It has only one eigenvalue
   d) It has all zero entries

Answer: b) It cannot be decomposed into smaller representations

21. The number of times an irreducible representation appears in a reducible representation is known as:
   a) The multiplicity
   b) The dimension
   c) The trace
   d) The eigenvalue

Answer: a) The multiplicity

22. In the process of reducing a reducible representation, one uses:
   a) The symmetry operations only
   b) The character table and orthogonality relations
   c) The eigenvalues of the matrices
   d) The molecular orbitals

Answer: b) The character table and orthogonality relations

23. A 1-dimensional representation is always:
   a) Irreducible
   b) Reducible
   c) Symmetric
   d) Orthogonal

Answer: a) Irreducible

24. The number of irreducible representations of a point group is equal to:
   a) The number of symmetry operations in the group
   b) The dimension of the largest representation
   c) The number of conjugacy classes in the group
   d) The sum of the dimensions of the representations

Answer: c) The number of conjugacy classes in the group

25. The character of a reducible representation for an operation is equal to:
   a) The product of the characters of its irreducible components
   b) The average of the characters of its irreducible components
   c) The sum of the characters of its irreducible components
   d) The difference of the characters of its irreducible components

Answer: c) The sum of the characters of its irreducible components

26. The process of reducing a representation involves:
   a) Determining the eigenvalues of the representation
   b) Finding the character table of the group
   c) Decomposing the representation into a sum of irreducible representations
   d) Calculating the symmetry operations

Answer: c) Decomposing the representation into a sum of irreducible representations

27. A representation with a character table having all non-zero entries is likely:
   a) Irreducible
   b) Reducible
   c) Trivial
   d) Singular

Answer: b) Reducible

28. The irreducible components of a reducible representation are:
   a) Unique to each group
   b) Always the same size
   c) The smallest possible representations
   d) Larger than the reducible representation

Answer: c) The smallest possible representations

29. In a reducible representation, the trace of the matrix for each symmetry operation:
   a) Is always zero
   b) Is the same for all operations
   c) Varies depending on the operation and representation
   d) Is equal to the dimension of the operation

Answer: c) Varies depending on the operation and representation

30. The orthogonality of irreducible representations is used to:
   a) Calculate the dimensions of the representations
   b) Identify the symmetry elements
   c) Determine the multiplicities of the irreducible components
   d) Reduce the representation to its components

Answer: d) Reduce the representation to its components

31. In group theory, the term "decomposition" refers to:
   a) Simplifying a matrix
   b) Identifying the irreducible components of a representation
   c) Increasing the size of a representation
   d) Calculating the character of a representation

Answer: b) Identifying the irreducible components of a representation

32. The character of the identity operation in any representation is equal to:
   a) The trace of the matrix
   b) The dimension of the representation
   c) Zero
   d) The number of symmetry operations

Answer: b) The dimension of the representation

33. In the context of irreducible representations, "degeneracy" refers to:
   a) The number of symmetry operations
   b) The number of identical irreducible representations
   c) The size of the representation
   d) The number of distinct eigenvalues

Answer: b) The number of identical irreducible representations

34. The number of distinct irreducible representations in a character table is equal to:
   a) The number of conjugacy classes
   b) The number of symmetry elements
   c) The number of dimensions of the reducible representation
   d) The number of operations in the group

Answer: a) The number of conjugacy classes

35. The process of finding a matrix representation of a group involves:
   a) Calculating the eigenvalues
   b) Decomposing the matrix into irreducible components
   c) Performing similarity transformations
   d) Identifying symmetry operations

Answer: d) Identifying symmetry operations

36. In a 2-dimensional representation, if the character for a particular symmetry operation is 0, the representation is:
   a) Always reducible
   b) Always irreducible
   c) Not necessarily irreducible
   d) Not well-defined

Answer: c) Not necessarily irreducible

37. The character table of a group helps in determining:
   a) The eigenvalues of matrices
   b) The multiplicities of irreducible representations
   c) The size of the group
   d) The symmetry of the molecule

Answer: b) The multiplicities of irreducible representations

38. The trace of a matrix in a reducible representation can be computed as:
   a) The sum of the eigenvalues
   b) The sum of the traces of the irreducible components
   c) The product of the dimensions of irreducible components
   d) The average of the eigenvalues

Answer: b) The sum of the traces of the irreducible components

39. The number of irreducible representations in a point group is equal to:
   a) The number of symmetry elements
   b) The number of irreducible components
   c) The number of conjugacy classes
   d) The number of dimensions

Answer: c) The number of conjugacy classes

40. To determine if a representation is reducible, one typically looks at:
   a) The eigenvalues
   b) The trace of the representation
   c) Whether it can be decomposed into smaller representations
   d) The size of the matrix

Answer: c) Whether it can be decomposed into smaller representations

41. The Great Orthogonality Theorem is a fundamental result in:
   a) Algebra
   b) Group Theory
   c) Number Theory
   d) Calculus

Answer: b) Group Theory

42. The Great Orthogonality Theorem provides conditions for:
   a) Diagonalization of matrices
   b) Decomposing a group into subgroups
   c) Orthogonality of irreducible representations
   d) Solving differential equations

Answer: c) Orthogonality of irreducible representations

43. According to the Great Orthogonality Theorem, irreducible representations of a group are:
   a) Always reducible
   b) Always orthogonal
   c) Not orthogonal
   d) Symmetric

Answer: b) Always orthogonal

44. The Great Orthogonality Theorem applies to:
   a) All representations of a group
   b) Only finite groups
   c) Only infinite groups
   d) Abelian groups only

Answer: b) Only finite groups

45. The Great Orthogonality Theorem helps in determining:
   a) The eigenvalues of matrices
   b) The dimensions of irreducible representations
   c) The symmetry of molecules
   d) The conjugacy classes of a group

Answer: b) The dimensions of irreducible representations

46. The orthogonality relations in the Great Orthogonality Theorem are used to:
   a) Simplify matrix operations
   b) Find irreducible components of representations
   c) Determine the symmetry of molecules
   d) Calculate vibrational frequencies

Answer: b) Find irreducible components of representations

47. In the context of the Great Orthogonality Theorem, the inner product of two distinct irreducible representations is:
   a) Always zero
   b) Equal to one
   c) Equal to the dimension of the group
   d) A function of the trace

Answer: a) Always zero

48. The Great Orthogonality Theorem is important for:
   a) Computing eigenvectors
   b) Analyzing molecular orbitals
   c) Classifying and analyzing group representations
   d) Solving linear equations

Answer: c) Classifying and analyzing group representations

49. According to the Great Orthogonality Theorem, the inner product of an irreducible representation with itself is:
   a) Equal to the order of the group
   b) The dimension of the group
   c) Equal to 1
   d) The number of conjugacy classes

Answer: d) The number of conjugacy classes

50. The Great Orthogonality Theorem asserts that the characters of irreducible representations are orthogonal with respect to:
   a) Symmetry operations
   b) Conjugacy classes
   c) Each other
   d) Molecular orbitals

Answer: c) Each other

51. The Great Orthogonality Theorem provides a method to:
   a) Determine the symmetry of a molecule
   b) Find the number of irreducible representations
   c) Calculate vibrational frequencies
   d) Solve polynomial equations

Answer: b) Find the number of irreducible representations

52. The orthogonality of irreducible representations is crucial for:
   a) Constructing molecular orbitals
   b) Performing group analysis
   c) Solving eigenvalue problems
   d) Determining the number of symmetry elements

Answer: b) Performing group analysis

53. The character of an irreducible representation of a group is:
   a) A matrix element
   b) The trace of the representation matrix
   c) The eigenvalue of the representation matrix
   d) The determinant of the representation matrix

Answer: b) The trace of the representation matrix

54. The orthogonality relations for irreducible representations involve:
   a) The order of the group
   b) The size of the matrices
   c) The dimensions of the representations
   d) The symmetry elements of the group

Answer: c) The dimensions of the representations

55. The Great Orthogonality Theorem implies that the matrix elements of distinct irreducible representations are:

a) Always equal
b) Orthogonal
c) Symmetric
d) Conjugate

Answer: b) Orthogonal

56. According to the Great Orthogonality Theorem, the product of two different irreducible representations' characters is:
    a) Always zero
    b) Equal to the trace of their product
    c) Equal to the dimension of the group
    d) Non-zero

Answer: a) Always zero

57. The Great Orthogonality Theorem aids in:
    a) Solving differential equations
    b) Finding molecular geometries
    c) Understanding the structure of the group
    d) Computing wavefunctions

Answer: c) Understanding the structure of the group

58. The Great Orthogonality Theorem is used to:
    a) Determine the number of symmetry elements
    b) Calculate the group order
    c) Verify the orthogonality of irreducible representations
    d) Identify the molecular orbitals

Answer: c) Verify the orthogonality of irreducible representations

59. The theorem provides a way to:
    a) Find eigenvalues
    b) Decompose complex matrices
    c) Check the orthogonality of representation matrices
    d) Compute vibrational modes

Answer: c) Check the orthogonality of representation matrices

60. The orthogonality relations in the Great Orthogonality Theorem are crucial for:
    a) Group classification
    b) Group decomposition
    c) Molecular modeling
    d) Solving algebraic equations

Answer: b) Group decomposition

61. The Great Orthogonality Theorem contributes to our understanding of:
    a) The dimensions of irreducible representations
    b) The vibrational modes of molecules
    c) The number of symmetry operations
    d) The order of the group

Answer: a) The dimensions of irreducible representations

62. The orthogonality of characters in the Great Orthogonality Theorem helps to:
    a) Calculate the eigenvalues of matrices
    b) Determine the dimensions of the group
    c) Identify and separate irreducible representations
    d) Find the molecular symmetry

Answer: c) Identify and separate irreducible representations

63. The orthogonality relations can be used to:
    a) Simplify the structure of molecular orbitals
    b) Calculate the bond angles in a molecule
    c) Compute the number of irreducible representations
    d) Find the trace of a matrix

Answer: c) Compute the number of irreducible representations

64. According to the Great Orthogonality Theorem, if two representations are orthogonal, their:
    a) Characters are equal
    b) Dimensions are the same
    c) Inner product is zero
    d) Eigenvalues are conjugate

Answer: c) Inner product is zero

65. The importance of the Great Orthogonality Theorem in spectroscopy is that it helps:
    a) Identify the number of energy levels
    b) Determine the symmetry of spectral transitions
    c) Compute molecular geometries
    d) Predict vibrational frequencies

Answer: b) Determine the symmetry of spectral transitions

66. The Great Orthogonality Theorem helps in:
    a) Group theoretical calculations
    b) Experimental observations
    c) Theoretical predictions
    d) Calculating eigenvalues

Answer: a) Group theoretical calculations

67. The theorem is essential for:
    a) Analyzing vibrational spectra
    b) Understanding molecular symmetry
    c) Computing bond energies
    d) Determining nuclear spin states

Answer: b) Understanding molecular symmetry

68. The orthogonality of representations means that:
    a) The characters are equal
    b) The product of the characters of two different irreducible representations is zero
    c) The dimensions are equal
    d) The matrix elements are symmetric

Answer: b) The product of the characters of two different irreducible representations is zero

69. In the Great Orthogonality Theorem, the number of irreducible representations of a group is equal to:
    a) The number of elements in the group
    b) The number of conjugacy classes in the group
    c) The order of the group
    d) The number of symmetry operations

Answer: b) The number of conjugacy classes in the group

70. The Great Orthogonality Theorem ensures that:
    a) All representations of a group are orthogonal
    b) Irreducible representations can be orthogonally decomposed
    c) Only reducible representations are orthogonal
    d) All symmetry operations are orthogonal

Answer: b) Irreducible representations can be orthogonally decomposed

71. The orthogonality of representation matrices allows for:
    a) Simplifying calculations in quantum mechanics
    b) Determining the number of symmetry operations
    c) Computing molecular geometries
    d) Classifying and analyzing group representations

Answer: d) Classifying and analyzing group representations

72. The Great Orthogonality Theorem is used to:
    a) Determine the frequency of vibrations in a molecule
    b) Decompose complex symmetry operations
    c) Identify and analyze group characters
    d) Calculate the bond lengths in a molecule

Answer: c) Identify and analyze group characters

73. The orthogonality of characters ensures that:
    a) All representations are reducible
    b) The product of characters from different irreducible representations is zero
    c) All matrices in a representation are diagonal
    d) The dimensions of representations are equal

Answer: b) The product of characters from different irreducible representations is zero

74. The Great Orthogonality Theorem helps in:
    a) Solving complex algebraic equations
    b) Determining the symmetry of complex molecules
    c) Computing the energy levels of a system

d) Identifying the vibrational modes

Answer: b) Determining the symmetry of complex molecules

75. The orthogonality relations are essential for:
    a) Simplifying experimental data
    b) Group theoretical analysis
    c) Solving for energy levels
    d) Predicting molecular interactions

Answer: b) Group theoretical analysis

76. In the Great Orthogonality Theorem, the inner product of the characters of the same irreducible representation is:
    a) Zero
    b) The number of conjugacy classes
    c) The dimension of the group
    d) Equal to one

Answer: b) The number of conjugacy classes

77. The theorem is a key tool for:
    a) Identifying the symmetry elements in a molecule
    b) Calculating the eigenvalues of matrices
    c) Analyzing and classifying the group representations
    d) Solving differential equations

Answer: c) Analyzing and classifying the group representations

78. The Great Orthogonality Theorem confirms that:
    a) All matrix elements of irreducible representations are equal
    b) The dimensions of irreducible representations are orthogonal
    c) The matrix elements of distinct irreducible representations are orthogonal
    d) All characters of a representation are identical

Answer: c) The matrix elements of distinct irreducible representations are orthogonal

79. According to the Great Orthogonality Theorem, the inner product of the characters of different irreducible representations is:
    a) Zero
    b) Equal to the order of the group
    c) The dimension of the irreducible representation
    d) Non-zero

Answer: a) Zero

80. The Great Orthogonality Theorem is crucial for:
    a) Finding the eigenvectors of a matrix
    b) Calculating the number of symmetry operations
    c) Identifying and analyzing irreducible representations
    d) Determining the molecular geometry

Answer: c) Identifying and analyzing irreducible representations

UNIT – 4

1. A character table provides information about:
    a) The symmetry of a molecule
    b) The group's elements
    c) The irreducible representations of a group
    d) The vibrational modes of a molecule

Answer: c) The irreducible representations of a group

2. In a character table, the rows typically represent:
    a) The symmetry operations
    b) The irreducible representations
    c) The molecular geometries
    d) The eigenvalues

Answer: b) The irreducible representations

3. The columns of a character table represent:
    a) The group's order
    b) The symmetry elements
    c) The conjugacy classes
    d) The molecular orbitals

Answer: c) The conjugacy classes

4. The diagonal elements in a character table for an irreducible representation correspond to:
    a) The group order
    b) The characters of the identity operation
    c) The number of symmetry elements
    d) The molecular vibration frequencies

Answer: b) The characters of the identity operation

5. The sum of the squares of the dimensions of the irreducible representations is equal to:
    a) The number of symmetry operations
    b) The number of elements in the group
    c) The number of molecular orbitals
    d) The number of conjugacy classes

Answer: b) The number of elements in the group

6. In a character table, the characters for a symmetry operation are:
    a) Always positive
    b) Always negative
    c) Complex numbers
    d) Real numbers

Answer: d) Real numbers

7. The characters of an irreducible representation for the identity operation are equal to:
    a) The order of the group
    b) The dimension of the representation
    c) Zero
    d) The number of symmetry operations

Answer: b) The dimension of the representation

8. Character tables are used to:
    a) Predict molecular vibrations
    b) Determine the symmetry properties of molecular orbitals
    c) Identify the symmetry of a molecule
    d) Calculate bond angles

Answer: c) Identify the symmetry of a molecule

9. The character of a representation for a symmetry operation is:
    a) The trace of the representation matrix
    b) The determinant of the representation matrix
    c) The eigenvalue of the representation matrix
    d) The sum of the eigenvalues

Answer: a) The trace of the representation matrix

10. The product of the characters for two irreducible representations is:
    a) Always zero
    b) Always positive
    c) Zero if the representations are different
    d) The same as the number of symmetry operations

Answer: c) Zero if the representations are different

11. To decompose a reducible representation into irreducible representations, one uses:
    a) The Great Orthogonality Theorem
    b) The Cauchy Integral Formula
    c) The Schur's Lemma
    d) The Jordan Canonical Form

Answer: a) The Great Orthogonality Theorem

12. The number of irreducible representations in a character table is equal to:
    a) The number of symmetry operations
    b) The number of conjugacy classes
    c) The number of symmetry elements
    d) The order of the group

Answer: b) The number of conjugacy classes

13. The character table can be used to:
    a) Calculate vibrational frequencies
    b) Predict electronic transitions
    c) Determine the symmetry labels of molecular orbitals
    d) Measure bond strengths

Answer: c) Determine the symmetry labels of molecular orbitals

14. The character of an irreducible representation for a symmetry operation reflects:
    a) The eigenvalue of the symmetry operation
    b) The dimension of the matrix representation
    c) The symmetry of the operation
    d) The trace of the matrix representation

Answer: d) The trace of the matrix representation

15. The number of characters in a character table row is equal to:
    a) The number of elements in the group
    b) The number of symmetry operations
    c) The number of conjugacy classes
    d) The number of irreducible representations

Answer: c) The number of conjugacy classes

16. In a character table, each entry represents:
    a) A matrix element
    b) The trace of a matrix
    c) The number of symmetry operations
    d) The number of irreducible components

Answer: b) The trace of a matrix

17. The character table for a given point group helps in:
    a) Calculating bond lengths
    b) Analyzing vibrational spectra
    c) Identifying molecular geometries
    d) Predicting the number of molecular orbitals

Answer: b) Analyzing vibrational spectra

18. The characters for different irreducible representations are orthogonal with respect to:
    a) The group's order
    b) The number of symmetry operations
    c) The number of conjugacy classes
    d) The number of dimensions

Answer: c) The number of conjugacy classes

19. In a character table, the representation with the character 1 for all operations is:
    a) The totally symmetric representation
    b) The totally antisymmetric representation
    c) The irreducible representation with the highest dimension
    d) The trivial representation

Answer: d) The trivial representation

20. The process of using a character table to analyze a molecule's symmetry involves:

a) Assigning symmetry labels to molecular orbitals
b) Determining the vibrational frequencies
c) Calculating bond strengths
d) Measuring bond angles

Answer: a) Assigning symmetry labels to molecular orbitals

21. The number of different irreducible representations of a group corresponds to:
    a) The number of symmetry operations
    b) The number of conjugacy classes
    c) The number of elements in the group
    d) The number of molecular orbitals

Answer: b) The number of conjugacy classes

22. The trace of a representation matrix for a symmetry operation is called:
    a) The character of the representation
    b) The eigenvalue of the matrix
    c) The dimension of the matrix
    d) The determinant of the matrix

Answer: a) The character of the representation

23. Character tables can be used to determine:
    a) The molecular weight
    b) The electronic configurations
    c) The symmetry properties of vibrational modes
    d) The bond lengths

Answer: c) The symmetry properties of vibrational modes

24. The symmetry of a molecule's vibrational modes can be determined using:
    a) The Great Orthogonality Theorem
    b) Character tables
    c) The Cauchy Integral Formula
    d) Schur's Lemma

Answer: b) Character tables

25. To find the symmetry species of vibrational modes, one must:
    a) Analyze the character table of the molecule's point group
    b) Calculate the bond angles
    c) Measure the infrared spectra
    d) Determine the molecular weight

Answer: a) Analyze the character table of the molecule's point group

26. In character tables, the sum of the characters in each column is:
    a) Always zero
    b) Equal to the group order
    c) Equal to the number of symmetry operations
    d) Equal to the dimension of the representation

Answer: b) Equal to the group order

27. The number of entries in each row of a character table equals:
    a) The number of elements in the group
    b) The number of conjugacy classes
    c) The number of irreducible representations
    d) The number of symmetry operations

Answer: b) The number of conjugacy classes

28. Character tables are essential for:
    a) Determining bond lengths
    b) Analyzing electronic spectra
    c) Calculating vibrational spectra
    d) Determining the symmetry properties of molecular orbitals

Answer: d) Determining the symmetry properties of molecular orbitals

29. When using a character table, the symmetry of a molecule can be used to:
    a) Predict the reactivity
    b) Assign symmetry labels to molecular orbitals
    c) Calculate bond strengths
    d) Determine the vibrational frequencies

Answer: b) Assign symmetry labels to molecular orbitals

30. To find the irreducible representations of a group, one must:
    a) Analyze its character table
    b) Measure bond angles
    c) Calculate vibrational frequencies
    d) Determine the molecular weight

Answer: a) Analyze its character table

31. The character table helps in identifying:
    a) The number of electrons in a molecule
    b) The symmetry elements of a molecule
    c) The types of molecular bonds
    d) The shape of the molecule

Answer: b) The symmetry elements of a molecule

32. In a character table, the character for a symmetry operation is the trace of the:
    a) Identity matrix
    b) Symmetry operation matrix
    c) Bonding matrix
    d) Molecular orbital matrix

Answer: b) Symmetry operation matrix

33. To find the symmetry labels of molecular orbitals, you need to:
    a) Use the character table of the molecule's point group
    b) Measure the bond angles
    c) Calculate the bond strengths
    d) Determine the molecular weight

Answer: a) Use the character table of the molecule's point group

34. The dimension of a representation in a character table is:
    a) The number of symmetry elements
    b) The number of conjugacy classes
    c) The number of characters in the row
    d) The order of the group

Answer: c) The number of characters in the row

35. The character of a representation for a particular symmetry operation is obtained by:
    a) Adding the eigenvalues
    b) Taking the trace of the representation matrix
    c) Calculating the determinant of the matrix
    d) Measuring the bond strengths

Answer: b) Taking the trace of the representation matrix

36. In a character table, the irreducible representations are:
    a) Always the same size
    b) Always orthogonal
    c) Always reducible
    d) Different for each molecule

Answer: b) Always orthogonal

37. The number of irreducible representations can be found by:
    a) Counting the rows in the character table
    b) Measuring the vibrational frequencies
    c) Analyzing the bond angles
    d) Determining the molecular geometry

Answer: a) Counting the rows in the character table

38. Character tables are used in:
    a) Molecular orbital theory
    b) Quantum chemistry
    c) Spectroscopy
    d) All of the above

Answer: d) All of the above

39. The number of irreducible representations corresponds to the number of:
    a) Symmetry operations
    b) Symmetry elements
    c) Conjugacy classes
    d) Molecular orbitals

Answer: c) Conjugacy classes

40. In a character table, the number of characters for each irreducible representation is:
   a) Equal to the group order
   b) Equal to the number of symmetry operations
   c) Equal to the number of conjugacy classes
   d) Equal to the number of molecular orbitals

Answer: c) Equal to the number of conjugacy classes

41. The character of a reducible representation can be used to:
   a) Determine the dimensions of the irreducible representations
   b) Calculate the molecular weights
   c) Predict bond angles
   d) Measure vibrational frequencies

Answer: a) Determine the dimensions of the irreducible representations

42. The character of the irreducible representations helps to:
   a) Predict reaction mechanisms
   b) Analyze electronic transitions
   c) Decompose complex representations
   d) Measure bond strengths

Answer: c) Decompose complex representations

43. The total number of irreducible representations of a group can be found by:
   a) Summing the squares of the dimensions of each irreducible representation
   b) Counting the number of rows in the character table
   c) Measuring the bond angles
   d) Determining the molecular weight

Answer: a) Summing the squares of the dimensions of each irreducible representation

44. Character tables are particularly useful in:
   a) Predicting molecular shapes
   b) Determining the number of valence electrons
   c) Assigning symmetry labels to vibrations
   d) Measuring bond angles

Answer: c) Assigning symmetry labels to vibrations

45. The entries in a character table for a specific symmetry operation are:
   a) The same for all irreducible representations
   b) Always zero
   c) Specific to each irreducible representation
   d) Dependent on the molecular weight

Answer: c) Specific to each irreducible representation

46. Character tables can help to:
   a) Determine the bond lengths
   b) Calculate the symmetry of vibrational modes
   c) Measure the bond strengths
   d) Predict electronic spectra

Answer: b) Calculate the symmetry of vibrational modes

47. The character of a representation for a specific symmetry element is:
   a) Equal to the eigenvalue of that element
   b) Equal to the trace of the matrix representing that element
   c) The number of symmetry elements
   d) The dimension of the representation

Answer: b) Equal to the trace of the matrix representing that element

48. The character table is important for:
   a) Determining the symmetry properties of molecular orbitals
   b) Measuring bond angles
   c) Predicting the vibrational frequencies
   d) Calculating the molecular weights

Answer: a) Determining the symmetry properties of molecular orbitals

49. Each character table row represents:
   a) A specific symmetry element
   b) A specific molecular vibration
   c) An irreducible representation
   d) A specific symmetry operation

Answer: c) An irreducible representation

50. The character table helps to find:
   a) The number of bonding orbitals
   b) The number of non-bonding orbitals
   c) The symmetry properties of molecular vibrations
   d) The energy levels of electronic transitions

Answer: c) The symmetry properties of molecular vibrations

51. Symmetry and point group theory are primarily used in spectroscopy to:
   a) Determine molecular geometries
   b) Predict vibrational spectra
   c) Calculate molecular weights
   d) Measure bond strengths

Answer: b) Predict vibrational spectra

52. The point group of a molecule helps in:
   a) Determining its electronic configuration
   b) Predicting its vibrational frequencies
   c) Calculating bond angles
   d) Identifying its symmetry elements

Answer: d) Identifying its symmetry elements

53. Which of the following spectroscopy techniques uses symmetry to analyze vibrational modes?
   a) NMR spectroscopy
   b) UV-Vis spectroscopy
   c) Infrared (IR) spectroscopy
   d) Mass spectrometry

Answer: c) Infrared (IR) spectroscopy

54. The selection rules for vibrational spectroscopy are determined by:
   a) The molecule's mass
   b) The symmetry properties of the molecule
   c) The bond strengths
   d) The molecular weight

Answer: b) The symmetry properties of the molecule

55. In the context of spectroscopy, the symmetry of a molecule affects:
   a) The color of the molecule
   b) The intensity of spectral lines
   c) The energy levels of molecular orbitals
   d) The molecular geometry

Answer: b) The intensity of spectral lines

56. Point group theory is used in spectroscopy to:
   a) Predict the number of peaks in a spectrum
   b) Determine the symmetry of electronic transitions
   c) Calculate the chemical shift in NMR
   d) Measure the bond strengths

Answer: b) Determine the symmetry of electronic transitions

57. The character of a vibration in IR spectroscopy can be predicted using:
   a) The molecule’s point group
   b) The bond length
   c) The mass of the atoms
   d) The molecular weight

Answer: a) The molecule’s point group

58. Symmetry considerations in Raman spectroscopy help to:
   a) Predict the presence of bonding orbitals
   b) Determine the vibrational modes that are active
   c) Measure bond angles
   d) Identify molecular weights

Answer: b) Determine the vibrational modes that are active

59. The point group of a molecule influences its:
   a) Electronegativity

b) Rotational spectra
c) Spectral intensity
d) Bond lengths

Answer: c) Spectral intensity

60. The selection rules for Raman spectroscopy are based on:
    a) The symmetry of the molecule
    b) The bond strengths
    c) The molecular weight
    d) The electronic configuration

Answer: a) The symmetry of the molecule

61. In vibrational spectroscopy, the number of active vibrations can be predicted by:
    a) The number of symmetry operations
    b) The point group of the molecule
    c) The molecular weight
    d) The bond lengths

Answer: b) The point group of the molecule

62. Symmetry elements in a molecule influence:
    a) The energy levels of electrons
    b) The shape of the IR spectrum
    c) The vibrational frequencies
    d) The bond strengths

Answer: c) The vibrational frequencies

63. In IR spectroscopy, vibrations that lead to a change in the dipole moment are:
    a) Symmetry-forbidden
    b) Not observed
    c) Active
    d) Invisible

Answer: c) Active

64. Raman spectroscopy is sensitive to:
    a) Changes in bond strengths
    b) Changes in polarizability
    c) Changes in molecular mass
    d) Changes in molecular weight

Answer: b) Changes in polarizability

65. Which spectroscopy technique relies on changes in polarizability?
    a) NMR spectroscopy
    b) UV-Vis spectroscopy
    c) Raman spectroscopy
    d) Mass spectrometry

Answer: c) Raman spectroscopy

66. The point group of a molecule can be used to:
    a) Predict the number of peaks in an NMR spectrum
    b) Assign vibrational modes to spectral peaks
    c) Calculate the bond angles
    d) Determine the molecular weight

Answer: b) Assign vibrational modes to spectral peaks

67. Symmetry considerations in electronic spectroscopy help to:
    a) Predict the intensity of spectral lines
    b) Determine the number of vibrational modes
    c) Calculate the chemical shifts
    d) Measure bond strengths

Answer: a) Predict the intensity of spectral lines

68. The number of vibrational modes in a molecule can be determined by:
    a) The symmetry of the molecule
    b) The point group of the molecule
    c) The mass of the atoms
    d) The bond lengths

Answer: b) The point group of the molecule

69. Point group theory helps in determining which vibrational modes are:
    a) Symmetry-forbidden
    b) Visible in UV-Vis spectra
    c) Active in IR or Raman spectra
    d) Detected by mass spectrometry

Answer: c) Active in IR or Raman spectra

70. The intensity of spectral lines in IR spectroscopy is related to:
    a) The mass of the atoms
    b) The molecular weight
    c) The change in dipole moment
    d) The bond lengths

Answer: c) The change in dipole moment

71. For a vibrational mode to be Raman active, it must:
    a) Change the dipole moment
    b) Change the polarizability
    c) Change the bond strength
    d) Change the molecular mass

Answer: b) Change the polarizability

72. The symmetry of a molecule can affect the:
    a) Color of the molecule
    b) Spectral lines' positions and intensities
    c) Bond lengths
    d) Chemical reactivity

Answer: b) Spectral lines' positions and intensities

73. To predict IR active vibrations, one should:
    a) Analyze the molecule's point group
    b) Measure bond strengths
    c) Calculate vibrational frequencies
    d) Determine the molecular weight

Answer: a) Analyze the molecule's point group

74. The point group of a molecule influences:
    a) Its IR and Raman activity
    b) The number of electrons
    c) The bond lengths
    d) The electronic configuration

Answer: a) Its IR and Raman activity

75. In which spectroscopy technique is symmetry used to determine selection rules for transitions?
    a) NMR spectroscopy
    b) UV-Vis spectroscopy
    c) Mass spectrometry
    d) X-ray diffraction

Answer: b) UV-Vis spectroscopy

76. Symmetry considerations are crucial for understanding:
    a) Nuclear magnetic resonance
    b) Electronic transitions
    c) Mass-to-charge ratios
    d) Bond dissociation energies

Answer: b) Electronic transitions

77. The symmetry of a molecule can be used to:
    a) Predict the number of peaks in an IR spectrum
    b) Assign symmetry labels to electronic transitions
    c) Measure bond angles
    d) Determine the molecular weight

Answer: b) Assign symmetry labels to electronic transitions

78. In IR spectroscopy, the vibrational modes that are active are determined by:
    a) The molecule’s polarizability
    b) The molecule’s symmetry elements
    c) The molecular weight
    d) The bond strengths

Answer: b) The molecule’s symmetry elements

79. The symmetry of molecular vibrations affects:
    a) The molecule’s color
    b) The number of IR peaks
    c) The number of Raman peaks
    d) The vibrational frequencies

Answer: d) The vibrational frequencies

80. Symmetry considerations are used in spectroscopy to:
   a) Predict the bond lengths
   b) Determine the molecule's symmetry labels
   c) Measure the molecular weights
   d) Calculate the vibrational frequencies

Answer: b) Determine the molecule's symmetry labels

81. In Raman spectroscopy, which of the following vibrational modes is active?
   a) Modes that change the dipole moment
   b) Modes that change the polarizability
   c) Modes that affect bond strengths
   d) Modes that alter the molecular weight

Answer: b) Modes that change the polarizability

82. The point group symmetry helps in:
   a) Assigning peaks in a UV-Vis spectrum
   b) Determining which vibrations are Raman or IR active
   c) Measuring bond dissociation energies
   d) Calculating chemical shifts in NMR

Answer: b) Determining which vibrations are Raman or IR active

83. In UV-Vis spectroscopy, symmetry considerations are used to:
   a) Predict bond angles
   b) Assign electronic transitions
   c) Measure bond strengths
   d) Determine molecular weights

Answer: b) Assign electronic transitions

84. Which spectroscopy technique involves symmetry to determine vibrational modes that can be observed?
   a) NMR spectroscopy
   b) Mass spectrometry
   c) Raman spectroscopy
   d) X-ray crystallography

Answer: c) Raman spectroscopy

85. The intensity of IR spectral lines is influenced by:
   a) The symmetry of the molecule
   b) The vibrational frequency
   c) The change in dipole moment
   d) The bond lengths

Answer: c) The change in dipole moment

86. In character tables, the irreducible representations help to:
   a) Predict the number of peaks in a UV-Vis spectrum
   b) Determine which vibrational modes are IR or Raman active
   c) Calculate the bond strengths
   d) Measure the molecular weight

Answer: b) Determine which vibrational modes are IR or Raman active

87. The point group of a molecule provides information on:
   a) The number of symmetry elements
   b) The number of vibrational modes
   c) The selection rules for vibrational and electronic transitions
   d) The bond strengths

Answer: c) The selection rules for vibrational and electronic transitions

88. The symmetry of molecular vibrations determines:
   a) The number of electronic transitions
   b) The intensity of the peaks in IR and Raman spectra
   c) The molecular geometry
   d) The bond angles

Answer: b) The intensity of the peaks in IR and Raman spectra

89. To determine the IR activity of vibrational modes, one must:
   a) Analyze the molecule's symmetry
   b) Measure bond strengths
   c) Calculate the vibrational frequencies
   d) Determine the molecular weight

Answer: a) Analyze the molecule's symmetry

90. Symmetry considerations are essential in spectroscopy to:
   a) Calculate the molecular weight
   b) Assign the correct peaks in a spectrum
   c) Measure bond lengths
   d) Determine chemical reactivity

Answer: b) Assign the correct peaks in a spectrum

91. The use of symmetry in spectroscopy allows for:
   a) Calculation of vibrational frequencies
   b) Prediction of the symmetry of molecular orbitals
   c) Determination of which vibrations are observable
   d) Measurement of bond strengths

Answer: c) Determination of which vibrations are observable

92. In Raman spectroscopy, the symmetry of a molecule influences:
   a) The color of the molecule
   b) The number of observable vibrational modes
   c) The molecular weight
   d) The bond dissociation energies

Answer: b) The number of observable vibrational modes

93. The point group of a molecule is used to:
   a) Calculate the intensity of spectral lines
   b) Predict which vibrational modes are active in IR and Raman spectroscopy
   c) Measure bond strengths
   d) Determine the molecular geometry

Answer: b) Predict which vibrational modes are active in IR and Raman spectroscopy

94. In IR spectroscopy, modes that lead to a change in the dipole moment are:
   a) Raman active
   b) Invisible
   c) IR active
   d) Not observed

Answer: c) IR active

95. The Great Orthogonality Theorem is used to:
   a) Predict spectral lines in IR and Raman spectra
   b) Determine the irreducible representations in a point group
   c) Measure bond angles
   d) Calculate vibrational frequencies

Answer: b) Determine the irreducible representations in a point group

96. The symmetry of electronic transitions can be predicted using:
   a) Character tables
   b) Vibrational frequencies
   c) Bond strengths
   d) Molecular weights

Answer: a) Character tables

97. In IR spectroscopy, vibrational modes that are inactive are typically those:
   a) That lead to a change in the dipole moment
   b) That do not affect the polarizability
   c) That affect bond lengths
   d) That alter the molecular weight

Answer: b) That do not affect the polarizability

98. The point group analysis helps to:
   a) Measure the bond strengths
   b) Predict the presence of spectral peaks
   c) Assign vibrational modes to spectral features
   d) Determine the molecular mass

Answer: c) Assign vibrational modes to spectral features

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