P.G. Sem. IInd Core course – VI Unit – III
Inorg. chem.

Point Groups and Character Table

Symmetry operations and matrices :-
In which we will see how the symm operations change the co-ordinates of a molecule and i is the effect of combining two or more symmetry operations.

Let us consider the effect of the operations on the co-ordinates of a C_{2v} molecule H_2O.
On performing E operation x, y and z rem unchanged.

$$x \xrightarrow{E} x$$
$$y \xrightarrow{E} y$$
$$z \xrightarrow{E} z$$

On performing C_2, σ_{xz} and σ_{yz} operation fol effects will arise —

$$\begin{matrix} x \\ y \\ z \end{matrix} \xrightarrow{C_2} \begin{matrix} -x \\ -y \\ z \end{matrix} \qquad \begin{matrix} x \\ y \\ z \end{matrix} \xrightarrow{\sigma_{xz}} \begin{matrix} +x \\ -y \\ z \end{matrix} \qquad \begin{matrix} x \\ y \\ z \end{matrix} \xrightarrow{\sigma_{yz}}$$

Combination of two operations can be sh as following -

$$\begin{matrix} x \\ y \\ z \end{matrix} \xrightarrow{C_2} \begin{matrix} -x \\ -y \\ z \end{matrix} \xrightarrow{\sigma_{xz}} \begin{matrix} -x \\ y \\ z \end{matrix}$$

Another way of representing the operation is in the form of matrices.

representation of the matrix will be as follows :
with n number of columns and m number of rows.

$$
\begin{array}{l c}
 & \begin{array}{cccccc} \text{1st column} & \text{2nd col.} & \text{3rd} & & & \end{array} \\
\begin{array}{l} \text{1st row} \\ \text{2nd row} \\ \text{3rd row} \\ \text{4th row} \\ \\ \end{array} &
\left[\begin{array}{cccccc}
a_{11} & a_{12} & a_{13} & a_{14} & \cdots & a_{1n} \\
a_{21} & a_{22} & a_{23} & a_{24} & & a_{2n} \\
a_{31} & a_{32} & a_{33} & a_{34} & \cdots & a_{3n} \\
 & & & & & \\
a_{m1} & a_{m2} & a_{m3} & a_{m4} & & a_{mn}
\end{array}\right]
\end{array}
$$

$m \times n$ matrix

m - row
n - column.

Square Matrix → If the number of row (m) is equal to the number of column (n), matrix is called Square matrix.

Representation of elements in the matrix →
An element a_{ij}, ~~represent~~ belongs to i^{th} row and j^{th} column.

a_{ij} — i → row, j → column

a_{23} — 2 → row, 3 → column

Digonal matrix → The elements which have $i = j$ are situated on the digonal ~~matrix~~ of the matrix and are called digonal matrix. For example a_{11}, a_{22}, a_{33} are digonal elements.

Unit matrix → The matrices in which ~~all~~ ~~elem~~ digonal elements are 1 and other elements are zero, are called unit matrices. For example

$$
\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}_{3\times 3}
$$

Unit matrix.

~~Sometimes~~ Some matrix have only one ~~row~~ column ~~and~~ or only one ~~column~~ row. These are called only single column or single row matrices. The vectors are ~~represented~~ normally represented as single column matrices and hence single column matrices are called vector matrix.

The combination (multiplication) of two matrices is carried out in the following way →

$$\begin{bmatrix} 2 & 1 \\ 0 & 3 \end{bmatrix} \times \begin{bmatrix} 4 & 2 \\ 3 & 1 \end{bmatrix} = \begin{bmatrix} 2\times4+1\times3 & 2\times2+1\times1 \\ 0\times4+3\times3 & 0\times2+3\times1 \end{bmatrix}$$

$$= \begin{bmatrix} 11 & 5 \\ 9 & 3 \end{bmatrix}$$

(Combination of matrices are possible only if the number of row in one are equal to number of column in another

Representation of symm. operations in the matrix form
⟶ . Symm. operations can be represented as matrix in the following way.

$$\begin{bmatrix} E \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} x \\ y \\ z \end{bmatrix}, \quad \begin{bmatrix} C_2 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} -x \\ -y \\ z \end{bmatrix}$$

↳ column matrix

combination of the single column matrix with E leaves it unchanged. Hence the matrix representation of E must be

$$E = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}.$$

Combination can be shown as follows —

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} (x\times1)+(y\times0)+(z\times0) \\ (x\times0)+(y\times1)+(z\times0) \\ (x\times0)+(y\times0)+(z\times0) \end{bmatrix} = \begin{bmatrix} x \\ y \\ z \end{bmatrix}$$

Matrix representation of other operations can be similarly worked out.

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$$[C_2]\begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} -x \\ -y \\ z \end{bmatrix} \quad \text{hence } C_2 = \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

similarly —

$$\sigma_{v\,xz}\begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} x \\ -y \\ z \end{bmatrix} \text{ hence } \sigma_{xz} \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad \text{and } \sigma_{yz} = \begin{bmatrix} -1 & 0 & 0 \\ 0 & 1 & 1 \\ 0 & 0 & 1 \end{bmatrix}$$

Character → The summation of the digonal elements of matrix is called as charater. Thus characker of the matrices of the different operations in C_{2v} point symmetry are.

E	C_2	$\sigma_{v\,xz}$	$\sigma_{v\,yz}$	← operations
3	−1	1	1	Characker

combination of two operations can be shown as the combination of their matrices →

$$C_2 \times \sigma_{v\,xz} = \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \times \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix} = \begin{bmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

i.e. $\sigma_{v\,yz}$.

combination of different matrices can be shown in the form of ~~ta~~ table →

Table

	E	C_2	$\sigma_{v\,xz}$	$\sigma_{v\,yz}$
E	E	C_2	$\sigma_{v\,xz}$	$\sigma_{v\,yz}$
C_2	C_2	E	$\sigma_{v\,yz}$	$\sigma_{v\,xz}$
$\sigma_{v\,xz}$	$\sigma_{v\,xz}$	$\sigma_{v\,yz}$	E	C_2
$\sigma_{v\,yz}$	$\sigma_{v\,yz}$	$\sigma_{v\,xz}$	C_2	E

The symm operations can be considered as elements. Thus molecules can be considered to be a set of elem...