Section B (Advanced Inorganic Chemistry: 422 Ch.) [40 MARKS]

Q1) Deduce the character table for the C_{2v} point group [15 Marks].

The answer:

Symmetry operations of this point group (C_{2v}) are: E, C_2, σ(xz), and σ'(yz). Let us suppose a point (x,y,z) on a Cartesian axes. We will see the effect of the symmetry operations on this point and from this we can deduce the matrix representation for each symmetry operation.

E:

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

C_2:

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

σ(xz):

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

σ'(yz):

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

So that x transforms under the following symmetry operation as:

	E	C_2	σ(xz)	σ'(yz)					
X:	1	-1	1	-1					

Hence, we say that x function forms a basis for the irreducible representation B_1

y transforms under the following symmetry operation as:

	E	C_2	σ(xz)	σ'(yz)					
y:	1	-1	-1	1					

Hence, we say that y function forms a basis for the irreducible representation B_2

And z transforms under the following symmetry operation as:

	E	C_2	σ(xz)	σ'(yz)					
z:	1	1	1	1					

Hence, we say that z function forms a basis for the irreducible representation A_1

So that A_1, B_1, and B_2 are the irreducible representations of point group C_{2v}. However, the number of symmetry operations in this group is 4. Therefore, there is still one missing irreducible representation.

We can find the missing one by finding out the product of each two irreducible representation and which is different from the already obtained one.

We can easily find that the missing irreducible representation is the one which its basis function is xy

And xy transforms under the following symmetry operation as:

	E	C_2	σ(xz)	σ'(yz)					
xy:	1	1	-1	-1					

Therefore, the character table for the point group C_{2v} will be as follows:

C_{2v}	E	C_2	σ(xz)	σ'(yz)		
A_1	1	1	1	1	z	
A_2	1	1	-1	-1		xy
B_1	1	-1	1	-1	x	
B_2	1	-1	-1	1	y	

Q2- Assign the point groups for <u>25 compounds only</u> of the following [25 Marks]:

The answer:

Compound	Point group	Compound	Point group
1	C_{2v}	16	D_{5d}
2	D_{5h}	17	D_{2h}
3	C_{2v}	18	D_{4h}
4	C_{3v}	19	C_s
5	C_{2v}	20	C_{2v}
6	D_{4h}	21	D_{3h}
7	C_{3v}	22	C_i
8	C_s	23	D_{3d}
9	C_{2v}	24	C_2
10	O_h	25	C_s
11	C_{4v}	26	C_s
12	C_{2v}	27	C_{2h}
13	C_{2h}	28	C_{2v}
14	D_{3h}	29	C_{3v}
15	C_2	30	D_{3h}