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Programme : M.Sc. Chemistry

Course Title : Physical Chemistry–I
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Unit-I Group Theory

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Construction of character Table

(i) Let's generate for the C_{2v} point group based on the above rules,

$$C_{2V} = \{ E, C_2, \sigma_v , \sigma_v' \}$$

Order of the group = 4
No. of classes = 4

The number of irreducible representations of a group is equal to the number of classes in the group.

C_{2v}	E	C_2	σ_v	σ_v'
Γ_1	d_1	?	?	?
Γ_2	d_2	a	b	c
Γ_3	d_3	d	e	f
Γ_4	d_4	g	h	i

The first representation is always the *totally symmetric* representation in which all characters are +1.

The sum of the squares of the dimensions of the irreducible representations of a group is equal to the order of the group (h).

$$d_1^2 + d_2^2 + d_3^2 + d_4^2 = h = 4$$

$$d_1^2 = 1$$

$$d_2^2 + d_3^2 + d_4^2 = 3$$

$$d_2 = d_3 = d_4 = 1$$

C_{2v}	E	C_2	σ_v	σ_v'
Γ_1	1	1	1	1
Γ_2	1	a	b	c
Γ_3	1	d	e	f
Γ_4	1	g	h	i

($\chi(\Gamma_1)$=+1)

Two different irreducible representations are orthogonal. The sum of the products of the characters for each symmetry operation is zero.

(row 1 * row 2)

- 1 + a + b + c = 0
- a + b + c = -1
- a = 1; b = c = -1 (others possible)

C_{2v}	E	C_2	σ_v	σ_v'
Γ_1	1	1	1	1
Γ_2	1	1	-1	-1
Γ_3	1	d	e	f
Γ_4	1	g	h	i

(row 2 * row 3)

- 1 + d - e - f = 0
- d - e - f = -1
- d = f = -1; e = +1 (others possible)

C_{2v}	E	C_2	σ_v	σ_v'
Γ_1	1	1	1	1
Γ_2	1	1	-1	-1
Γ_3	1	-1	1	-1
Γ_4	1	g	h	i

Two different irreducible representations are orthogonal. The sum of the products of the characters for each symmetry operation is zero.

(row 3 * row 4)

- 1 - g + h - i = 0
- - g + h - i = -1
- g = h = -1; i = +1

C_{2v}	E	C_2	σ_v	σ_v'
Γ_1	1	1	1	1
Γ_2	1	1	-1	-1
Γ_3	1	-1	1	-1
Γ_4	1	-1	-1	1

Two different irreducible representations are orthogonal. The sum of the products of the characters for each symmetry operation is zero.

The sum of the squares of the characters in any irreducible representation equal to the order of the group(h).

C_{2v}	E	C_2	σ_v	σ_v'
Γ_1	1	1	1	1
Γ_2	1	1	-1	-1
Γ_3	1	-1	1	-1
Γ_4	1	-1	-1	1

Mulliken symbols for irreps:

- "A"—symmetric *wrt* rotation about principle axis ($\chi[C_n(z)] = +1$)
- "B"— irrep is antisymmetric *wrt* rotation about the principle axis ($\chi[C_n(z)] = -1$)

For C_{2v}:

C_{2v}	E	C_2	σ_v	σ_v'
A_1	1	1	1	1
A_2	1	1	-1	-1
B_1	1	-1	1	-1
B_2	1	-1	-1	1